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The Reduced Overall Wiener Index

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Abstract

Motivation. Comparison with the overall Wiener index, a novel set of overall Wiener indexes (^{m}RW, $^{m}RW_{p}$, $^{m}RW_{pc}$, and $^{m}RW_{c}$) were defined, which named the reduced overall Wiener indexes. The potential usefulness of the reduced overall Wiener indexes in QSAR/QSPR is evaluated by its correlation with a number of C3-C8 alkanes and by a favorable comparison with models based on the overall Wiener index and molecular connectivity indexes. This can extend the usefulness of the Wiener number, and can make the Wiener number to be a kind of widely used topological index in practice.

Method. The present communication attempts to correlate boiling point, surface tension, critical Temperature and critical pressures of 38 diverse functional acyclic compounds with the reduced overall Wiener indices and to compare those with relations of the overall Wiener index and molecular connectivity indices to explore the diagnostic

Results. The results show that considerably better statistics is obtained when using the reduced overall Wiener index. The reduced overall Wiener indexes provided even the same statistical results as the molecular connectivity indexes in all models with five variables, and the standard deviations provided by these two sets of indexes are rather closed.

Conclusions. Summarized the results, one may conclude that the reduced overall Wiener index examined shows a good potential for QSAR and QSPR studies. It denotes some information of molecular structure, and make up for the pitfalls of Wiener index. This can extend the usefulness of the Wiener number, and can make the Wiener number to be a kind of widely used topological index in practice.

Keywords. Wiener index; reduced overall Wiener index; molecular connectivity index; Quantitative structure–property relationships; QSPR; topological index; molecular graph.

Abbreviations and notations

MLR, multiple linear regression	QSAR, quantitative structure-activity relationships
QSPR, quantitative structure-property relationships	$^{m}RW_{t}$, notations of the reduced overall Wiener indexes

1 INTRODUCTION

The Wiener number W(G), one of widely used descriptors of molecular topology, was introduced in 1947 by Wiener[1] as the path number for saturated acyclic hydrocarbons. The path number was defined as the number of the bonds between all pairs of non-hydrogen atoms in the molecule[2]. The Wiener number W(G) =W of a structure G is equal to the half-sum of distances of the distance matrix between all pairs of vertices[3-4]:

$$W(G) = W = \frac{1}{2}\sum_{i}\sum_{j} d_{ij} \tag{1}$$

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Recently, Bonchev proposes a new approach to the topological characterization of molecules[5-7]. It proceeds from the total number of subgraphs *K(G)* of molecular graph *G* and their presentation in complete series of classes of order *e*, with *e*=0,1,2,…, E being the constant number of edges in each subgraph of a certain class, and E being the number of edges in the entir graph. He use the Wiener numbers of each subgraph, extending thus that seminal molecular descriptor to its most complete version, the overall Wiener index[8]. In this study, according to this approach we defined a reduced overall Wiener index.

2 MATERIALS AND METHODS

According to the definition of Bonchev[8], the overall Wiener indexes are defined as follows:

Definition 1. The overall Wiener index *OW(G)* of any graph *G* is defined as the sum of the Wiener indices $W_i(G_i)$ of all *K* subgraphs of *G*:

$$OW(G) = \sum_{i=1}^{K} W_i(G_i \subset G) \tag{2}$$

Definition 2. The *e*th-order overall Wiener index ${}^eOW(G)$ of any graph G is defined as the sum of the Wiener indices $W_j({}^eG_j)$ of all ${}^eK$ subgraphs ${}^eG_j \subset G$ that have e edges:

$${}^eOW(G) = \sum_{j=1}^{{}^eK} W_j({}^eG_j \subset G) \tag{3}$$

Definition 3. The *e*th-order overall Wiener index ${}^eOW(G)$ can be presented as a sum of terms, ${}^eOW_k(G)$, representing the sum of the Wiener indices in the subgraphs of specified type. For acyclic graphs these are the path (*k*=*p*), cluster(*k*=*c*), and pathcluster (*k*=*pc*) type, as defined by Kier and Hall[9]:

$${}^eOW(G) = {}^eOW_p(G) + {}^eOW_c(G) + {}^eOW_{pc}(G) = \sum_{j=1}^{{}^eK_p} W_{pj} + \sum_{l=1}^{{}^eK_p} W_{cl} + \sum_{m=1}^{{}^eK_p} W_{pcm} \tag{4}$$

Definition 4. The overall Wiener index vector *OW'(G)* of any graph *G* is the sequence of all ${}^eOW(G)$s listed in an ascending order of the number of edges *e*:

$$OW'(G) = OW\{{}^0OW, \quad {}^1OW, \quad {}^2OW, \quad \cdots, \quad {}^EOW\} \tag{5}$$

or in more detail for acyclic graphs:

$$OW'(G) = OW\{{}^0OW, \quad {}^1OW, \quad {}^2OW, \quad {}^3OW_p, \quad {}^3OW_c, \quad \cdots, {}^EOW_p, \quad {}^EOW_c, \quad {}^EOW_{pc}\} \tag{6}$$

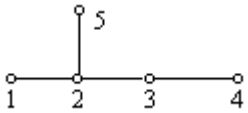
When we get the overall Wiener indexes ${}^eOW$ and ${}^eOW_k$, we can define the reduced overall Wiener indexes ${}^eRW$ and ${}^eRW_k$, they are defied as:

$${}^eRW = \frac{{}^eOW}{N^2} \tag{7}$$

$${}^eRW_k = \frac{{}^eOW_k}{N^2} \tag{8}$$

Where *N* is the number of atoms (except hydrogen) of molecules.

Example:



e=1: 1-2, 2-3, 3-4, 2-5; ${}^{1}RW = (4\times1)/5^2 = 0.16$

e=2: 1-2-3, 2-3-4, 1-2-5, 5-2-3; ${}^{2}RW = (4\times4)/5^2 = 0.64$

e=3: 1-2-3-4, 5-2-3-4, 1-2-3-5; ${}^{3}RW = (2\times10 + 9)/5^2 = 1.16$

e=3: the entire graph; ${}^{4}RW = 18/5^2 = 0.72$

RW =0.16+0.64+1.16+0.72 = 2.68; RW'= 2.68 (0.16, 0.64, 1.16, 0.72)

Table 1. Reduced overall Wiener index RW, and its eth-order components, calculated for C3-C8 alkanes

no	Molecule	${}^{1}RW$	${}^{2}RW$	${}^{3}RW$	${}^{4}RW$	${}^{5}RW$	${}^{6}RW$	${}^{7}RW$	RW
1	propane	0.2222	0.444	0.000	0.000	0.000	0.000	0.000	0.667
2	n-butane	0.1875	0.500	0.625	0.000	0.000	0.000	0.000	1.313
3	2-methyl propane	0.1875	0.750	0.563	0.000	0.000	0.000	0.000	1.500
4	n- pentane	0.1600	0.480	0.800	0.800	0.000	0.000	0.000	2.240
5	2- methyl butane	0.1600	0.640	1.160	0.720	0.000	0.000	0.000	2.680
6	2,2-dimethyl propane	0.1600	0.960	1.440	0.640	0.000	0.000	0.000	3.200
7	n-hexane	0.1389	0.444	0.833	1.111	0.972	0.000	0.000	3.500
8	2- methyl pentane	0.1389	0.556	1.083	1.611	0.889	0.000	0.000	4.278
9	3- methyl pentane	0.1389	0.556	1.361	1.556	0.861	0.000	0.000	4.472
10	2,3-dimethyl butane	0.1389	0.667	1.611	2.000	0.806	0.000	0.000	5.222
11	2,2-dimethyl butane	0.1389	0.778	1.833	1.944	0.778	0.000	0.000	5.472
12	n- heptane	0.1224	0.408	0.816	1.224	1.429	1.143	0.000	5.143
13	2- methyl hexane	0.1224	0.490	1.000	1.592	2.082	1.061	0.000	6.347
14	3- methyl hexane	0.1224	0.490	1.204	1.959	2.000	1.020	0.000	6.796
15	3-ethyl pentane	0.1224	0.490	1.408	2.327	1.898	0.980	0.000	7.224
16	2,4-dimethyl pentane	0.1224	0.571	1.184	2.367	2.612	0.980	0.000	7.837
17	2,3-dimethyl pentane	0.1224	0.571	1.592	2.653	2.510	0.939	0.000	8.388
18	2,2-dimethyl pentane	0.1224	0.653	1.551	2.653	2.531	0.939	0.000	8.449
19	3,3-dimethyl pentane	0.1224	0.653	1.959	2.939	2.408	0.898	0.000	8.980
20	2,2,3-trimethyl butane	0.1224	0.735	2.143	3.633	2.918	0.857	0.000	10.408
21	n-octane	0.1094	0.375	0.781	1.250	1.641	1.750	1.313	7.219
22	2- methyl heptane	0.1094	0.438	0.922	1.531	2.141	2.563	1.234	8.938
23	3- methyl heptane	0.1094	0.438	1.078	1.813	2.625	2.469	1.188	9.719
24	4- methyl heptane	0.1094	0.438	1.078	2.125	2.578	2.438	1.172	9.938
25	3-ethylhexane	0.1094	0.438	1.234	2.406	3.047	2.313	1.125	10.672
26	2,5-dimethyl hexane	0.1094	0.500	1.063	1.813	3.188	3.250	1.156	11.078
27	2,4-dimethyl hexane	0.1094	0.500	1.219	2.406	3.578	3.125	1.109	12.047
28	2,2-dimethyl exane	0.1094	0.563	1.344	2.344	3.578	3.156	1.109	12.203
29	2,3-dimethyl hexane	0.1094	0.500	1.375	2.656	3.516	3.094	1.094	12.344
30	3,4-dimethyl hexane	0.1094	0.500	1.531	2.938	3.938	3.000	1.063	13.078
31	2-methyl-3-ethyl pentane	0.1094	0.500	1.531	3.250	3.875	2.938	1.047	13.250
32	3,3-dimethyl hexane	0.1094	0.563	1.656	3.188	3.891	2.969	1.047	13.422
33	3-methyl-3-ethyl pentane	0.1094	0.563	1.969	3.719	4.219	2.813	1.000	14.391
34	2,2,4-trimethyl pentane	0.1094	0.625	1.484	3.250	4.938	3.688	1.031	15.125
35	2,3,4-trimethyl pentane	0.1094	0.563	1.672	3.500	4.844	3.625	1.016	15.328
36	2,2,3-trimethyl pentane	0.1094	0.625	1.953	4.000	5.188	3.531	0.984	16.391
37	2,3,3-trimethyl pentane	0.1094	0.625	2.109	4.250	5.109	3.469	0.969	16.641
38	2,2,3,3-tetramethyl butane	0.1094	0.750	2.531	5.563	6.703	3.938	0.906	20.500

Table 2. Path (=p), cluster(c), and path cluster (pc) terms of reduced overall Wiener index of C3-C8 alkanes

no.	Molecule	${}^{3}RW_p$	${}^{3}RW_c$	${}^{4}RW_p$	${}^{4}RW_c$	${}^{4}RW_{pc}$	${}^{5}RW_p$	${}^{5}RW_c$	${}^{5}RW_{pc}$	${}^{6}RW_p$	${}^{6}RW_c$	${}^{6}RW_{pc}$	${}^{7}RW_p$	${}^{7}RW_c$	${}^{7}RW_{pc}$

1	propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	n-butane	0.6250	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	2-methyl propane	0.0000	0.5625	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	n- pentane	0.8000	0.0000	0.8000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	2- methyl butane	0.8000	0.3600	0.0000	0.0000	0.7200	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	2,2-dimethyl propane	0.0000	1.4400	0.0000	0.6400	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7	n-hexane	0.8333	0.0000	1.1111	0.0000	0.0000	0.9722	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
8	2- methyl pentane	0.8333	0.2500	1.1111	0.0000	0.5000	0.0000	0.0000	0.8889	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
9	3- methyl pentane	1.1111	0.2500	0.5556	0.0000	1.0000	0.0000	0.0000	0.8611	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10	2,3-dimethyl butane	1.1111	0.5000	0.0000	0.0000	2.0000	0.0000	0.8056	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
11	2,2-dimethyl butane	0.8333	1.0000	0.0000	0.4444	1.5000	0.0000	0.0000	0.7778	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
12	n- heptane	0.8163	0.0000	1.2245	0.0000	0.0000	1.4286	0.0000	0.0000	1.1429	0.0000	0.0000	0.0000	0.0000	0.0000
13	2- methyl hexane	0.8163	0.1837	1.2245	0.0000	0.3673	1.4286	0.0000	0.6531	0.0000	0.0000	1.0612	0.0000	0.0000	0.0000
14	3- methyl hexane	1.0204	0.1837	1.2245	0.0000	0.7347	0.7143	0.0000	1.2857	0.0000	0.0000	1.0204	0.0000	0.0000	0.0000
15	3-ethyl pentane	1.2245	0.1837	1.2245	0.0000	1.1020	0.0000	0.0000	1.8980	0.0000	0.0000	0.9796	0.0000	0.0000	0.0000
16	2,4-dimethyl pentane	0.8163	0.3673	1.6327	0.0000	0.7347	0.0000	0.0000	2.6122	0.0000	0.0000	0.9796	0.0000	0.0000	0.0000
17	2,3-dimethyl pentane	1.2245	0.3673	0.8163	0.0000	1.8367	0.0000	0.5918	1.9184	0.0000	0.0000	0.9388	0.0000	0.0000	0.0000
18	2,2-dimethyl pentane	0.8163	0.7347	1.2245	0.3265	1.1020	0.0000	0.0000	2.5306	0.0000	0.0000	0.9388	0.0000	0.0000	0.0000
19	3,3-dimethyl pentane	1.2245	0.7347	0.4082	0.3265	2.2041	0.0000	0.0000	2.4082	0.0000	0.0000	0.8980	0.0000	0.0000	0.0000
20	2,2,3-trimethyl butane	1.2245	0.9184	0.0000	0.3265	3.3061	0.0000	1.7755	1.1429	0.0000	0.8571	0.0000	0.0000	0.0000	0.0000
21	n-octane	0.7813	0.0000	1.2500	0.0000	0.0000	1.6406	0.0000	0.0000	1.7500	0.0000	0.0000	1.3125	0.0000	0.0000
22	2- methyl heptane	0.7813	0.1406	1.2500	0.0000	0.2813	1.6406	0.0000	0.5000	1.7500	0.0000	0.8125	0.0000	0.0000	1.2344
23	3- methyl heptane	0.9375	0.1406	1.2500	0.0000	0.5625	1.6406	0.0000	0.9844	0.8750	0.0000	1.5938	0.0000	0.0000	1.1875
24	4- methyl heptane	0.9375	0.1406	1.5625	0.0000	0.5625	1.0938	0.0000	1.4844	0.8750	0.0000	1.5625	0.0000	0.0000	1.1719
25	3-ethylhexane	1.0938	0.1406	1.5625	0.0000	0.8438	1.0938	0.0000	1.9531	0.0000	0.0000	2.3125	0.0000	0.0000	1.1250
26	2,5-dimethyl hexane	0.7813	0.2813	1.2500	0.0000	0.5625	2.1875	0.0000	1.0000	0.0000	0.0000	3.2500	0.0000	0.0000	1.1563
27	2,4-dimethyl hexane	0.9375	0.2813	1.5625	0.0000	0.8438	1.0938	0.0000	2.4844	0.0000	0.0000	3.1250	0.0000	0.0000	1.1094
28	2,2-dimethyl exane	0.7813	0.5625	1.2500	0.2500	0.8438	1.6406	0.0000	1.9375	0.0000	0.0000	3.1563	0.0000	0.0000	1.1094
29	2,3-dimethyl hexane	1.0938	0.2813	1.2500	0.0000	1.4063	1.0938	0.4531	1.9688	0.0000	0.0000	3.0938	0.0000	0.0000	1.0938
30	3,4-dimethyl hexane	1.2500	0.2813	1.2500	0.0000	1.6875	0.5469	0.4531	2.9375	0.0000	0.0000	3.0000	0.0000	0.0000	1.0625
31	2-methyl-3-ethyl pentane	1.2500	0.2813	1.5625	0.0000	1.6875	0.0000	0.4531	3.4219	0.0000	0.0000	2.9375	0.0000	0.0000	1.0469
32	3,3-dimethyl hexane	1.0938	0.5625	1.2500	0.2500	1.6875	0.5469	0.0000	3.3438	0.0000	0.0000	2.9688	0.0000	0.0000	1.0469
33	3-methyl-3-ethyl pentane	1.4063	0.5625	0.9375	0.2500	2.5313	0.0000	0.0000	4.2188	0.0000	0.0000	2.8125	0.0000	0.0000	1.0000
34	2,2,4-trimethyl pentane	0.7813	0.7031	1.8750	0.2500	1.1250	0.0000	0.0000	4.9375	0.0000	0.0000	3.6875	0.0000	0.0000	1.0313
35	2,3,4-trimethyl pentane	1.2500	0.4219	1.2500	0.0000	2.2500	0.0000	0.9063	3.9375	0.0000	0.0000	3.6250	0.0000	0.0000	1.0156
36	2,2,3-trimethyl pentane	1.2500	0.7031	0.9375	0.2500	2.8125	0.0000	1.3594	3.8281	0.0000	0.6563	2.8750	0.0000	0.0000	0.9844
37	2,3,3-trimethyl pentane	1.4063	0.7031	0.6250	0.2500	3.3750	0.0000	1.3594	3.7500	0.0000	0.6563	2.8125	0.0000	0.0000	0.9688
38	2,2,3,3-tetramethyl butane	1.4063	1.1250	0.0000	0.5000	5.0625	0.0000	4.0781	2.6250	0.0000	3.9375	0.0000	0.0000	0.9063	0.0000

3 RESULTS AND DISCUSSION

Wiener number has two pitfalls, one is it shows opposing complexity trends when used for a mixed set of isomeric and nonisomeric compounds, the other is its degeneracy[8]. These two pitfalls prevent the use of this number as a measure of molecular complexity. As the overall Wiener index preserves the basic features of the original Wiener number, and eliminating its pitfalls[8], our reduced overall Wiener number can also eliminating the pitfalls of Wiener number, and can be a good measure of molecular complexity.

The potential usefulness of the reduced overall Wiener index for structure-property and structure-activity studies can be evaluated by performing comparative modeling of reference [8] against overall Wiener index and molecular connectivity index, the most widely used molecular descriptors in QSAR/QSPR. In this study, we apply multiple linear regression analysis (MLR) in a QSPR

modeling of 4 physical properties of (C_3-C_8) alkanes. The properties are boiling point, bp in ºC; heats of vaporization, HV in KJ/mol; critical pressures, PC in atm; and surface tension, ST in dyn/cm (Table 3.)[10]. Some of the models of molecular connectivity are taken from Bonchev[8], the best models of the reduced overall Wiener index have been selected from the computer program.

The reduced overall Wiener indices of the 38 molecules are shown in Table 1 and Table 2, and the physical properties of theirs are shown in Table 3. Table 4 summarizes the statistics (correlation coefficient r^2, standard deviation s, and the Fischer ratio F) of the molecular connectivity, overall Wiener and reduced overall Wiener index models of the C_3-C_8 alkanes.

Table 3. Experimental values for the physical properties of the 38 alkanes

no.	Molecule	bp	HV	PC	ST
1	propane	-42.070		42.01	
2	n-butane	-0.500		37.47	
3	2-methyl propane	-11.730		36.00	
4	n- pentane	36.074	115.205	33.31	16.00
5	2- methyl butane	27.852	116.426	32.90	15.00
6	22dimethyl propane	9.503	122.074	31.57	
7	n-hexane	68.740	130.688	29.92	18.42
8	2- methyl pentane	60.271	131.933	29.95	17.38
9	3- methyl pentane	63.282	129.717	30.83	18.12
10	23-dimethyl butane	57.988	130.240	30.99	17.37
11	22-dimethyl butane	49.741	132.744	30.67	16.30
12	n- heptane	98.427	146.540	27.01	20.26
13	2- methyl hexane	90.052	147.656	27.20	19.29
14	3- methyl hexane	91.850	145.821	28.10	19.79
15	3-ethyl pentane	93.475	143.517	28.60	20.44
16	24-dimethyl pentane	80.500	148.949	27.40	18.15
17	23-dimethyl pentane	89.784	144.153	29.20	19.96
18	22-dimethyl pentane	79.197	148.695	28.40	18.02
19	33-dimethyl pentane	86.064	144.530	30.00	19.59
20	223-trimethyl butane	80.882	145.191	29.75	18.76
21	n-octane	125.665	162.592	24.64	21.76
22	2- methyl heptane	117.647	163.663	24.80	20.60
23	3- methyl heptane	118.925	161.832	25.60	21.17
24	4- methyl heptane	117.709	162.105	25.60	21.17
25	3-ethylhexane	118.534	160.072	25.74	21.51
26	25-dimethyl hexane	109.103	164.697	25.00	19.73
27	24-dimethyl hexane	109.429	163.093	25.80	20.05
28	22-dimethyl exane	106.840	164.285	25.60	19.60
29	23-dimethyl hexane	115.607	160.395	26.60	20.99
30	34-dimethyl hexane	117.725	158.814	27.40	21.64
31	2-methyl-3-ethyl pentane	115.650	158.794	27.40	21.52
32	33-dimethyl hexane	111.969	160.879	27.20	20.63
33	3-methyl-3-ethyl pentane	118.259	157.026	28.90	21.99
34	224-trimethyl pentane	99.238	165.083	25.50	18.77
35	234-trimethyl pentane	113.467	158.852	27.60	21.14
36	223-trimethyl pentane	109.841	159.526	28.20	20.67
37	233-trimethyl pentane	114.760	157.292	29.00	21.56
38	2233-tetramethyl butane	106.470		24.50	

The comparison of the three columns of Table 4 shows that considerably better statistics results are obtained by the reduced overall Wiener index models. The reduced overall Wiener indexes

provided even the same statistics results as the molecular connectivity indexes in all models with five variables, and the standard deviations provided by these two sets of indexes are rather close.

Table 4. Comparison of multi linear regression statistics (correlation coefficient, standard deviation, and the Fischer ratio) for the C3-C8 alkane properties models with 5 parameters produced by three sets of topological indexes.

Number of index	r^2	s	F
	Boiling Point		
Overall Wiener index	0.9904	4.36	659
Molecular connectivity index	0.9959	2.86	1541
Reduced overall Wiener index	0.9967	2.57	1903
	HV		
Overall Wiener index	0.9942	0.40	959
Molecular connectivity index	0.9979	0.24	2704
Reduced overall Wiener index	0.9922	0.46	715
	Critical Pressure		
Overall Wiener index	0.9901	0.40	638
Molecular connectivity index	0.9666	0.73	185
Reduced overall Wiener index	0.9944	0.30	1131
	Surface Tension		
Overall Wiener index	0.9916	0.18	639
Molecular connectivity index	0.9848	0.24	349
Reduced overall Wiener index	0.9929	0.16	752

The best models of reduced overall Wiener with five variables obtained for the 4 examined alkane properties are give below. The first order reduced overall Wiener index takes part in all models.

$$\text{bp} = 281.9489 - 1320.9429\,{}^{1}RW - 67.3448\,{}^{2}RW + 3.0811\,{}^{6}RW_p + 4.9362\,{}^{7}RW + 3.5261\,{}^{4}RW_{pc} \quad (9)$$
$$n = 38,\ r = 0.9967,\ s = 2.57,\ F = 1903$$
$$\text{HV} = 70.6730 - 230.7699\,{}^{1}RW - 13.6419\,{}^{2}RW - 0.8525\,{}^{4}RW_p + 0.8143\,{}^{7}RW + 0.4780\,{}^{6}RW_p \quad (10)$$
$$n = 34,\ r = 0.\ 9922,\ s = 0.46,\ F = 715$$
$$\text{PC} = 6.2186 + 175.6811\,{}^{1}RW + 2.6638\,{}^{3}RW + 0.6353\,{}^{4}RW_{pc} - 6.9741\,{}^{2}RW - 6.2478\,{}^{7}RW_c \quad (11)$$
$$n = 38,\ r = 0.\ 9944,\ s = 0.30,\ F = 1131$$
$$\text{ST} = 38.0850 - 90.0952\,{}^{1}RW + 2.2937\,{}^{3}RW - 17.7076\,{}^{2}RW - 0.9043\,{}^{4}RW_p - 0.3751\,{}^{5}RW_p \quad (12)$$
$$n = 33,\ r = 0.\ 9929,\ s = 0.16,\ F = 752$$

4 CONCLUSIONS

Summarized the results, one may conclude that the reduced overall Wiener indexes examined show a good potential for QSAR and QSPR studies. The results show that considerably better statistics is obtained when using reduced overall Wiener indexes. The reduced overall Wiener indexes provided even the same statistics results as the molecular connectivity indexes in all models with five variables, and the standard deviations provided by these two sets of indexes are rather closed. The reduced overall Wiener index can be a good measure of molecular complexity. This can extend the usefulness of the Wiener number, and can make the Wiener number to be a kind of

widely used topological index in practice.

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