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Brief communication

Predicting water solubility and octanol water partition coefficient for carbon nanotubes based on the chiral vector

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Abstract

Components of the chiral vector of carbon nanotubes have been examined in role of structural descriptors. Two-variable models of water solubility and octanol water partition coefficient calculated with components of the chiral vectors have quite good statistical characteristics. These are in case of the water solubility: $n = 8$, $r^2 = 0.99998$, $s = 0.05338$, $F = 126{,}611$ (training set); $n = 8$, $r^2 = 0.9999$, $s = 0.09329$, $F = 674{,}556$ (test set) and in case of octanol water partition coefficient: $n = 8$, $r^2 = 0.9991$, $s = 0.3664$, $F = 2927$ (training set); $n = 8$, $r^2 = 0.9996$, $s = 0.2870$, $F = 5928$ (test set).

Keywords: Carbon nanotubes; Chiral vector; Predictive modeling

1. Introduction

Quantitative Structure - Property/Activity Relationships (QSPR/QSAR) is one from branches of theoretical chemistry. Milestones of this branch of chemistry have been established in pioneer researches of H. Wiener (Wiener, 1947, 1948). Main idea of these studies is using of a molecular graph in calculation of special coefficients (descriptors) which can be correlated with physicochemical properties of organic compounds. From the beginning of 1970s, number of different descriptors conceptually analogical to Wiener number starts to increase (Hosoya, 1972; Amidon and Anik, 1976; Bonchev et al., 1980; Randic and Basak, 2001).

Carbon nanotubes (CNTs) are new class of substances. Since their discovery in 1991, there has been intensive research activity in the area of CNTs, not only because of their fascinating structural features and properties, but also because of their potential technological applications (Rao et al., 2001). Molecules of these substances contain hundreds or even thousands of atoms. Under such circumstances calculation of the "classic" descriptors becomes problematic.

Most available information on structure of the CNT is chiral vector (n, m) (Torrens, 2005). In fact, the components of chiral vector contain information about rolling up graphite layer in formation of CNT. Physicochemical behaviour of CNTs is correlated with numerical values of components of the chiral vector. For example, $m - n = 3k$ (k is an integer) is known to be a necessary criterion for conductivity in CNT (Ormsby and King, 2004).

The aim of the present study is an estimation of chiral vector as a base of modeling water solubility ($\log S$, S in mol/L) and

Table 1
Components of chiral vector, experimental and calculated values of water solubility, and octanol water partition coefficient for CNTs under consideration

No.	n	m	Log S_{expr}	Log S_{calc}	Log P_{expr}	Log P_{calc}
1[a]	9	0	−36.6	−36.6716	29.8	30.0134
2	10	0	−40.1	−40.1791	34.0	33.7837
3[a]	11	0	−43.6	−43.6866	37.9	37.5540
4[a]	12	0	−47.1	−47.1941	41.7	41.3243
5[a]	13	0	−50.7	−50.7016	45.4	45.0946
6	14	0	−54.2	−54.2091	49.1	48.8649
7	15	0	−57.7	−57.7166	52.7	52.6352
8[a]	16	0	−61.3	−61.2241	56.3	56.4055
9	17	0	−64.8	−64.7316	59.8	60.1758
10[a]	18	0	−68.4	−68.2391	63.6	63.9461
11	5	5	−40.7	−40.6121	32.3	32.9327
12[a]	6	6	−47.8	−47.7137	40.5	40.3031
13	7	7	−54.8	−54.8153	48.1	47.6735
14	8	8	−61.9	−61.9169	55.3	55.0439
15[a]	9	9	−69.0	−69.0185	62.5	62.4143
16	10	10	−76.1	−76.1201	69.6	69.7847

[a] CNTs of the test set.

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Table 2
Statistical characteristics of models

	Training set ($n = 8$)			Test set ($n = 8$)		
	r^2	s	F	r^2	s	F
Water solubility	0.99998	0.0534	126,611	0.99990	0.0933	67,456
Octanol water partition coefficient	0.99910	0.364	2,927	0.99960	0.287	5,928

octanol water partition coefficient (log P) of the CNTs. It is well-known, that the water solubility and the octanol water partition coefficient are parameters close related to toxicity (Netzeva and Schultz, 2005).

2. Method

In fact, numerical values of components of chiral vector are structural descriptors. Thus their numerical values can be used in multiple regression analysis (MRA) (Sengupta et al., 2004). Data on 16 CNTs was taken from literature (Torrens, 2005). These 16 CNTs have been randomly divided into training and test sets. The data is demonstrated in Table 1.

3. Results

Two-variable models of the water solubility and octanol water partition coefficient have been calculated by the least squares method. These models are the following

$$\log S = -5.1041 - 3.5075n - 3.5941m \quad (1)$$

$$\log P = -3.9193 + 3.7703n - 3.6001m \quad (2)$$

Statistical characteristics of these models calculated with Eqs. (1) and (2) are represented in Table 2. One can see from Table 2 that predictions of the water solubility and octanol water partition coefficient based on the components of the chiral vector are quite good. It is indicates that water solubility and octanol water partition coefficient of CNTs are determined by features of the rolling up of graphite layer.

4. Conclusions

Components of chiral vectors of nanotubes can be used in role of structural descriptors in multiple regression analysis aimed to predict numerical values of water solubility and octanol water partition coefficient of carbon nanotubes.

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