

# QSPR Analysis of Degree–Eccentricity Based Degcity Indices for Benzenoid Hydrocarbons

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## Abstract

This study examines the effectiveness of degcity indices based on degree and eccentricity in the QSPR analysis of benzenoid hydrocarbons. These indices incorporate both vertex degree and eccentricity to capture structural features of molecular graphs. Experimental physicochemical properties such as boiling point, molecular weight, and critical parameters are analyzed using linear regression models. The results indicate that the fourth degcity index shows the strongest predictive performance, while the first, second, and sixth indices also provide good correlations. Comparison with standard topological indices shows strong agreement, particularly with eccentricity-based measures. Overall, degcity indices demonstrate promising predictive capability and strong discriminating ability for molecular structures.

**Keywords:** Benzenoid Hydrocarbons; Degcity Indices; QSPR analysis; Topological Indices.

## 1. Introduction

Topological indices are numerical descriptors obtained from the graph representation of molecular structures [4, 13]. These indices have become essential tools in Quantitative Structure-Property Relationship (QSPR) studies, where they are used to model and predict physicochemical properties of chemical compounds. By converting structural information into numerical form, topological indices enable the development of mathematical relationships between molecular structure and observable properties.

QSPR modeling is widely recognized as an efficient and reliable approach for predicting physicochemical properties without requiring extensive experimental procedures [12, 13]. Several well-known topological indices, including Zagreb indices, Randić index, Harmonic index, Forgotten index, and eccentricity-based descriptors, have been successfully applied in QSPR studies. The benzenoid hydrocarbons considered in this study were selected from previously reported datasets available in the literature [1, 4, 6, 7, 10, 11, 14] due to the availability of experimentally measured physicochemical properties and their importance in mathematical chemistry and QSPR investigations. These compounds represent structurally diverse benzenoid systems, making them suitable for evaluating the predictive capability of the proposed degcity indices. Benzenoid hydrocarbons have been widely investigated in QSPR studies due to their structural diversity and the availability of experimentally measured physicochemical data [6, 7, 11, 14].

Traditional topological descriptors based exclusively on either vertex degree or eccentricity capture only limited aspects of molecular graph structure. Degree-based descriptors mainly capture local connectivity patterns, while eccentricity-based descriptors reflect global structural characteristics [15, 17]. In contrast, degcity indices integrate both degree and eccentricity information within a single framework, thereby simultaneously reflecting local and global structural characteristics of molecular graphs. This combined structural representation may enhance the discriminatory power and predictive effectiveness of degcity indices in QSPR modeling compared with conventional single-parameter descriptors.

In this work, linear regression analysis is employed to investigate the applicability of degcity indices for modeling the physicochemical properties of benzenoid hydrocarbons. The predictive performance of these indices is further compared with several established topological descriptors.

### 1.1. Preliminaries

Let  $G$  be a molecular graph with vertex set  $V(G)$  and edge set  $E(G)$ . For vertices  $u, v \in V(G)$ , let  $d(u)$  and  $d(v)$  denote their degrees, while  $e(u)$  and  $e(v)$  represent their eccentricities. Based on these parameters, the degcity indices are defined as follows [16]:

$$DC_1(G) = \sum_{e=uv \in E(G)} [e(u) + e(v)] [d(u) + d(v)]$$

$$DC_2(G) = \sum_{e=uv \in E(G)} \frac{e(u) + e(v)}{d(u) + d(v)}$$

$$DC_3(G) = \sum_{e=uv \in E(G)} \frac{d(u) + d(v)}{e(u) + e(v)}$$

$$DC_4(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{e(u) + e(v)}{d(u) + d(v)}}$$

$$DC_5(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d(u) + d(v)}{e(u) + e(v)}}$$

$$DC_6(G) = \sum_{e=uv \in E(G)} \frac{e(u) + e(v)}{d(u)d(v)}$$

$$DC_7(G) = \sum_{e=uv \in E(G)} \frac{d(u) + d(v)}{e(u)e(v)}$$

To assess their effectiveness, these indices are compared with several well-known topological descriptors such as Zagreb indices, Randić index, Harmonic index, Forgotten index, Geometric-Arithmetic index, Sum-connectivity index, and Eccentricity based indices.

**Definition 1.** The first and second Zagreb indices were introduced by I. Gutman and N. Trinajstić [5] and are defined as

$$M_1 = M_1(G) = \sum_{u \in V(G)} d_u^2,$$

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

**Definition 2.** The Randić index was introduced by Milan Randić [13] and is defined as

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

with summation going over all pairs of adjacent vertices of the molecular graph  $G$ .

**Definition 3.** The Forgotten index ( $F$ -index) was introduced by B. Furtula and Gutman [3] and is defined as

$$F = F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2).$$

**Definition 4.** The Harmonic index was introduced by S. Fajtlowicz [2] and is defined as

$$H = H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

**Definition 5.** The Geometric-Arithmetic index was introduced by D. Vukičević and B. Furtula [17] and is defined as

$$GA = GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

**Definition 6.** The Sum-Connectivity index was introduced by B. Zhou and N. Trinajstić [19] and is defined as

$$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

**Definition 7.** The first and second Zagreb eccentricity indices were introduced by D. Vukičević and A. Graovac [18] and are defined as

$$FZE = \xi_1(G) = \sum_{u \in V(G)} e_u^2,$$

$$SZE = \xi_2(G) = \sum_{uv \in E(G)} e_u e_v.$$

**Definition 8.** The eccentric-connectivity index was introduced by V. Sharma et al. [15] and is defined as

$$ECI = \xi^c(G) = \sum_{u \in V(G)} d_u e_u = \sum_{uv \in E(G)} (e_u + e_v).$$

## 2. QSPR analysis of degcity indices for benzenoid hydrocarbons

In this study, a dataset consisting of various benzenoid hydrocarbons is considered. The experimentally measured physicochemical properties include:

- Boiling Point (BP)
- Molecular Weight (MW)
- Critical Pressure (CP)
- Critical Temperature (CT)
- Critical Volume (CV)
- XLogP3
- Complexity (C)

These values are obtained from previously reported literature. Corresponding degcity indices for each compound are computed using their molecular graph representations.

The experimentally determined physicochemical properties of benzenoid hydrocarbons, including boiling point (BP), molecular weight (MW), critical pressure (CP), critical temperature (CT), critical volume (CV), XLogP3, and complexity (C), are presented in Table 1 and are adopted from [8, 11]. The computed degcity indices and well-known topological indices corresponding to these compounds are presented in Table 2 and Table 3 respectively. Additionally, representative molecular graphs of selected benzenoid hydrocarbons are illustrated in Figure 1.

**Table 1:** Experimental values of physicochemical properties for benzenoid hydrocarbons

Benzenoid hydrocarbons	BP (°C)	MW	CP	CT	CV	XLogP3	C
Benzene	80.1	78.11	47.69	323.79	263.5	2.1	15.5
Naphthalene	218	128.17	38.97	484.95	409.5	3.3	80.6
Anthracene	340	178.23	32.43	586.11	555.5	4.4	154
Phenanthrene	340	178.23	32.43	586.11	555.5	4.5	174
Tetracene	432	228.3	27.41	650.8	701.5	5.9	236
Benzo[c]phenanthrene	436.7	228.3	27.41	650.8	701.5	5.7	266
Benzo[a]anthracene	438	228.3	27.41	650.8	701.5	5.8	294
Chrysene	448	228.3	27.41	650.8	701.5	5.7	264
Triphenylene	438	228.3	27.41	650.8	701.5	4.9	217
Pyrene	404	202.25	30.73	625.65	619.5	4.9	217
Pentacene	524.6	278.3	23.47	714.53	847.5	6.7	325
Benzo[a]tetracene	547.5	278.3	23.47	714.53	847.5	6.7	399
Dibenzo[a,h]anthracene	524	278.3	23.47	714.53	847.5	6.5	361
Dibenzo[a,j]anthracene	524.7	278.3	23.47	714.53	847.5	6.5	363
Pentaphene	547.5	278.3	23.47	714.53	847.5	6.7	361
Benzo[g]chrysene	525	278.3	23.47	714.53	847.5	7.0	399
Benzo[c]chrysene	524.7	278.3	23.47	714.53	847.5	7.0	399
Picene	520	278.3	23.47	714.53	847.5	7.0	361
Benzo[b]chrysene	524.7	278.3	23.47	714.53	847.5	6.5	399
Dibenzo[a,c]anthracene	518	278.3	23.47	714.53	847.5	6.7	361
Perylene	400	252.3	26.08	689.17	765.5	5.8	304
Benzo[e]pyrene	467.5	252.3	26.08	689.17	765.5	6.4	336
Benzo[a]pyrene	495	252.3	26.08	689.17	765.5	6.0	372
Benzo[ghi]perylene	500	276.3	24.85	728.06	829.5	6.6	411
Hexacene	604	328.4	20.33	779.67	993.5	8.2	418
Coronene	525	300.4	23.7	767.68	893.5	7.2	376

**Table 2:** Computed degcity indices for benzenoid hydrocarbons

Benzenoid hydrocarbons	DC <sub>1</sub>	DC <sub>2</sub>	DC <sub>3</sub>	DC <sub>4</sub>	DC <sub>5</sub>	DC <sub>6</sub>	DC <sub>7</sub>
Benzene	144	9	4	7.3485	4.8990	9	13.5
Naphthalene	400	20.6	6.4349	14.8951	8.3122	19.3333	43.6
Anthracene	840	39.3333	7.0426	24.8343	10.5153	35.5555	114.8333

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Table 2 continued from previous page

Benzenoid hydrocarbons	$DC_1$	$DC_2$	$DC_3$	$DC_4$	$DC_5$	$DC_6$	$DC_7$
Phenanthrene	792	37.3333	7.4616	24.1912	10.8096	33.8888	102.5833
Tetracene	1424	63.5333	7.5327	36.1458	12.4539	56.2222	235.4
Benzo[c]phenanthrene	1222	55.3666	8.7450	33.7221	13.3885	49.4444	175.6
Benzo[a]anthracene	1356	60.7833	7.8920	35.3496	12.7422	53.9722	214.0666
Chrysene	1338	60.0666	8.0209	35.1211	12.8392	53.4444	209.1666
Triphenylene	1170	53.2	9.0306	33.0745	13.6245	47.6666	160.75
Pyrene	972	42.1333	9.2656	28.0169	13.1409	36.8888	114.5
Pentacene	2176	93.8666	7.7502	48.9258	14.0739	81.7777	421.8333
Benzo[a]tetracene	2092	90.6166	8.0558	48.0557	14.3414	79.1944	391.3
Dibenzo[a,h]anthracene	2058	89.4	8.2198	47.6923	14.4750	77.5833	381.2666
Dibenzo[a,j]anthracene	1948	84.8666	8.6176	46.5093	14.8254	74.4444	343.0666
Pentaphene	2076	90	8.1173	47.8936	14.3922	78.6666	386.05
Benzo[g]chrysene	1693	74.8333	9.9309	43.5989	15.8794	66.2222	262.7333
Benzo[c]chrysene	1898	83.0166	8.8783	45.9622	15.0310	73.0277	325.4666
Picene	2058	89.6	8.2198	47.7401	14.4684	78.6666	381.8666
Benzo[b]chrysene	2075	89.4	8.1374	47.7666	14.4151	76.9166	380.4333
Dibenzo[a,c]anthracene	1786	78.6333	9.4193	44.7061	15.4728	69.3888	291.15
Perylene	1404	59.8666	10.4212	37.5312	15.6591	52.1111	183.6
Benzo[e]pyrene	1314	54.7	10.4497	35.1282	15.3553	47	162.4333
Benzo[a]pyrene	1564	66.25	9.4748	39.4372	14.9245	57.4166	232.1333
Benzo[ghi]perylene	1638	66.5333	11.8118	41.9878	17.6936	56.5555	206.45
Hexacene	3078	129.8333	7.9552	62.8457	15.5703	111.8888	684
Coronene	1872	73.2	13.2024	46.4444	19.7281	61	229.3

Table 3: Computed values of well-known topological indices for benzenoid hydrocarbons

Molecule	$M_1$	$M_2$	R	GA	H	F	SCI	FZE	SZE	ECI
Benzene	24	24	3	6	3	48	3	54	54	36
Naphthalene	50	57	4.96632	10.9191	4.9333	118	5.1971	182	178	90
Anthracene	76	90	6.93265	15.8383	6.8666	188	7.3942	472	516	180
Phenanthrene	76	91	6.94948	15.8787	6.8999	188	7.408	424	459	170
Tetracene	102	123	8.89897	20.7575	8.7999	258	9.5913	970	1085	298
Benzo[c]phenanthrene	102	125	8.93265	20.8383	8.8666	258	9.6189	729	800	257
Benzo[a]anthracene	102	124	8.91581	20.7979	8.8333	258	9.6051	882	983	284
Chrysene	102	125	8.93265	20.8383	8.8666	258	9.6189	858	959	280
Triphenylene	102	128	8.85773	20.8787	8.8999	258	9.6327	660	729	246
Pyrene	94	117	7.93265	18.8383	7.8666	242	8.6189	499	534	203
Pentacene	128	156	10.8653	25.6767	10.7333	328	11.7884	1732	1982	448
Benzo[a]tetracene	128	157	10.88214	25.7171	10.7666	328	11.8022	1607	1832	431
Dibenzo[a,h]anthracene	128	158	10.89897	25.7575	10.7999	328	11.816	1562	1780	424
Dibenzo[a,j]anthracene	128	158	10.89897	25.7575	10.7999	328	11.816	1399	1584	402
Pentaphene	128	157	10.88214	25.7171	10.7666	328	11.8022	1588	1807	428
Benzo[g]chrysene	128	160	10.93265	25.8383	10.8666	328	11.8436	1080	1209	351
Benzo[c]chrysene	128	159	10.91581	25.7979	10.8333	328	11.8298	1339	1512	392
Picene	128	159	10.91581	25.7979	10.8333	328	11.8298	1562	1780	424
Benzo[b]chrysene	128	158	10.89897	25.7575	10.7999	328	11.816	1575	1793	426
Dibenzo[a,c]anthracene	128	159	10.91581	25.7979	10.8333	328	11.8298	1196	1344	370

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Table 3 continued from previous page

Molecule	$M_1$	$M_2$	R	GA	H	F	SCI	FZE	SZE	ECI
Perylene	120	152	9.93265	23.8383	9.8666	312	10.8436	758	862	286
Benzo[e]pyrene	116	147	9.41581	23.8383	9.8666	304	10.8436	676	774	265
Benzo[a]pyrene	120	151	9.91581	27.7979	9.8333	312	10.8298	943	1080	318
Benzo[ghi]perylene	138	178	10.91581	26.7979	10.8333	366	12.0546	856	995	326
Hexacene	154	189	12.83163	30.5959	12.6666	398	13.9855	2814	3255	626
Coronene	156	204	11.89897	29.7575	11.7999	420	13.2655	954	1128	366

## 2.1. Regression based QSPR modeling for benzenoid hydrocarbons

In the present work, simple linear regression analysis was employed as an initial and interpretable QSPR modeling approach to examine the relationship between degcity indices and physicochemical properties. Linear regression is widely used in preliminary QSPR studies because it provides direct insight into descriptor-property relationships and allows straightforward statistical interpretation of correlation trends. The general form of the model is:

$$P = c + (TI)m, \quad (1)$$

where  $P$  is the physicochemical property,  $TI$  is the topological index,  $m$  is the slope and  $c$  is the intercept. Using this model, separate regression equations are developed for each degcity index with respect to all considered properties.

### 1. $DC_1$ index [ $DC_1(G)$ ]:

$$\begin{aligned} BP &= 199.0234357 + [DC_1(G)]0.165207752 \\ MW &= 115.6271565 + [DC_1(G)]0.082826184 \\ CP &= 39.781137 - [DC_1(G)]0.00824972 \\ CT &= 464.8021651 + [DC_1(G)]0.130335092 \\ CV &= 370.9303117 + [DC_1(G)]0.241527481 \\ XLogP3 &= 2.875230457 + [DC_1(G)]0.001984352 \\ C &= 67.11396292 + [DC_1(G)]0.151484029 \end{aligned}$$

### 2. $DC_2$ index [ $DC_2(G)$ ]:

$$\begin{aligned} BP &= 186.6167238 + [DC_2(G)]3.983552372 \\ MW &= 110.7357913 + [DC_2(G)]1.977463179 \\ CP &= 40.41368756 - [DC_2(G)]0.19911305 \\ CT &= 457.6501709 + [DC_2(G)]3.103661169 \\ CV &= 355.691578 + [DC_2(G)]5.780872248 \\ XLogP3 &= 2.751972472 + [DC_2(G)]0.047466001 \\ C &= 58.96113126 + [DC_2(G)]3.604915006 \end{aligned}$$

### 3. $DC_3$ index [ $DC_3(G)$ ]:

$$\begin{aligned} BP &= 137.5229547 + [DC_3(G)]36.91154973 \\ MW &= 72.15638249 + [DC_3(G)]19.97175504 \\ CP &= 44.41643195 - [DC_3(G)]2.02468628 \\ CT &= 343.6812173 + [DC_3(G)]37.54386998 \\ CV &= 261.5130814 + [DC_3(G)]56.22647546 \\ XLogP3 &= 2.148699304 + [DC_3(G)]0.44194229 \\ C &= -30.5677671 + [DC_3(G)]38.63604784 \end{aligned}$$

### 4. $DC_4$ index [ $DC_4(G)$ ]:

$$\begin{aligned} BP &= 105.0029686 + [DC_4(G)]9.072267898 \\ MW &= 69.10109023 + [DC_4(G)]4.532541884 \\ CP &= 44.71129672 - [DC_4(G)]0.45911289 \\ CT &= 385.2817769 + [DC_4(G)]7.295577905 \\ CV &= 236.0824704 + [DC_4(G)]13.19587482 \\ XLogP3 &= 1.799554835 + [DC_4(G)]0.107581805 \\ C &= -20.2058282 + [DC_4(G)]8.347346375 \end{aligned}$$

### 5. $DC_5$ index [ $DC_5(G)$ ]:

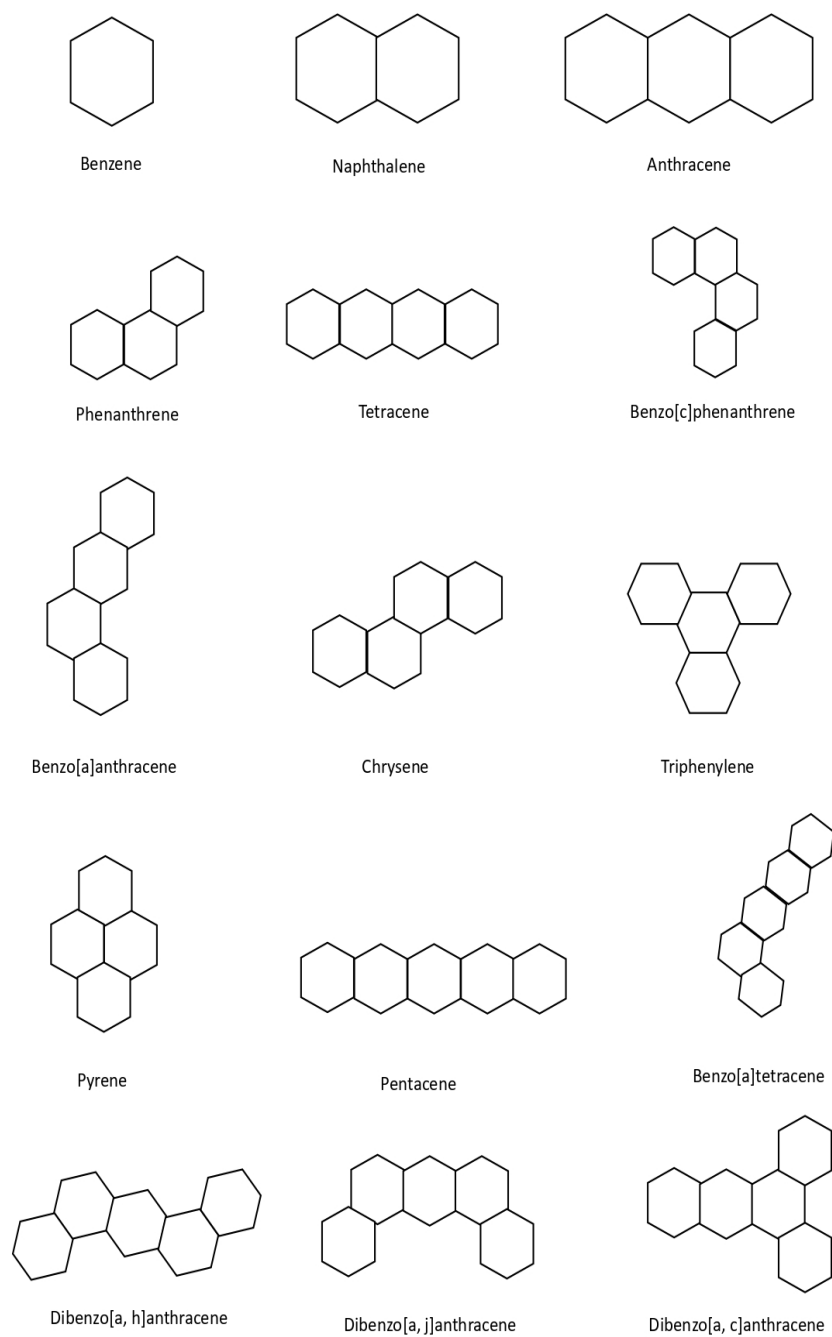
$$\begin{aligned} BP &= -9.9491118 + [DC_5(G)]33.71769041 \\ MW &= 3.89270579 + [DC_5(G)]17.4087453 \\ CP &= 51.45428818 - [DC_5(G)]1.77336066 \\ CT &= 249.091004 + [DC_5(G)]30.2827978 \\ CV &= 56.85651629 + [DC_5(G)]49.91415613 \\ XLogP3 &= 0.442947795 + [DC_5(G)]0.399362027 \\ C &= -151.924902 + [DC_5(G)]32.90285986 \end{aligned}$$

### 6. $DC_6$ index [ $DC_6(G)$ ]:

$$\begin{aligned} BP &= 180.5457264 + [DC_6(G)]4.652920387 \\ MW &= 108.367961 + [DC_6(G)]2.298818773 \\ CP &= 40.72690449 - [DC_6(G)]0.23273576 \\ CT &= 454.1142146 + [DC_6(G)]3.604983107 \\ CV &= 348.3066195 + [DC_6(G)]6.728145065 \\ XLogP3 &= 2.690535178 + [DC_6(G)]0.055257473 \\ C &= 55.10305501 + [DC_6(G)]4.18299195 \end{aligned}$$

### 7. $DC_7$ index [ $DC_7(G)$ ]:

$$\begin{aligned} BP &= 293.9299523 + [DC_7(G)]0.632584403 \\ MW &= 164.0878855 + [DC_7(G)]0.313702247 \\ CP &= 34.87980785 - [DC_7(G)]0.03095418 \\ CT &= 546.2088064 + [DC_7(G)]0.473501065 \\ CV &= 510.5955432 + [DC_7(G)]0.921233505 \\ XLogP3 &= 3.9973906 + [DC_7(G)]0.007667701 \\ C &= 158.9852286 + [DC_7(G)]0.561070754 \end{aligned}$$



**Figure 1:** Molecular graph representations of selected benzenoid hydrocarbons considered in the present study.

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The statistical parameters of linear regression model for the degcity indices  $DC_1$ ,  $DC_2$ ,  $DC_3$ ,  $DC_4$ ,  $DC_5$ ,  $DC_6$  and  $DC_7$  are listed in Table 4, 5, 6, 7, 8, 9 and 10 respectively, where  $r$  = correlation coefficient,  $SE$  = standard error,  $F$  = F-test and  $SF$  = significance F.

**Table 4:** Statistical parameters of the linear regression model for  $DC_1(G)$

Property	c	m	r	SE	F	SF
BP	199.0234357	0.165207752	0.915764857	46.06178234	124.7222	$5.44995 \times 10^{-11}$
MW	115.6271565	0.082826184	0.936237734	19.75692065	170.3966695	$2.14719 \times 10^{-12}$
CP	39.781137	-0.00824972	-0.89044548	2.679819056	91.88221	$1.11628 \times 10^{-9}$
CT	464.8021651	0.130335092	0.869856174	46.97927737	74.62329	$7.8962 \times 10^{-9}$
CV	370.9303117	0.241527481	0.941045004	55.18369783	185.7273	$8.59492 \times 10^{-13}$
XLogP3	2.875230457	0.001984352	0.938077593	0.46576406	175.9826196	$1.52563 \times 10^{-12}$
C	67.11396292	0.151484029	0.885599458	50.49458423	87.25863174	$1.82859 \times 10^{-9}$

**Table 5:** Statistical parameters of the linear regression model for  $DC_2(G)$

Property	c	m	r	SE	F	SF
BP	186.6167238	3.983552372	0.910446938	47.42754986	116.28	$1.10473 \times 10^{-10}$
MW	110.7357913	1.977463179	0.921631793	21.82041909	135.3680124	$2.36352 \times 10^{-11}$
CP	40.41368756	-0.19911305	-0.88613231	2.728943702	87.74769	$1.73389 \times 10^{-9}$
CT	457.6501709	3.103661169	0.854065039	49.53733059	64.70068	$2.86568 \times 10^{-8}$
CV	355.691578	5.780872248	0.928683586	60.50035622	150.4861	$7.91084 \times 10^{-12}$
XLogP3	2.751972472	0.047466001	0.925194948	0.510222142	142.6501077	$1.37777 \times 10^{-11}$
C	58.96113126	3.604915006	0.868952586	53.80459993	73.99061937	$8.53818 \times 10^{-9}$

**Table 6:** Statistical parameters of the linear regression model for  $DC_3(G)$

Property	c	m	r	SE	F	SF
BP	137.5229547	36.91154973	0.572384611	94.02190244	11.69432	0.002246106
MW	72.15638249	19.97175504	0.631548684	43.59614812	15.9237284	0.00053977
CP	44.41643195	-2.02468628	-0.61136159	4.659910796	14.32415	0.000906119
CT	343.6812173	37.54386998	0.700966464	67.92009254	23.18409	$6.64765 \times 10^{-5}$
CV	261.5130814	56.22647546	0.61285371	128.9043963	14.43626	0.00087312
XLogP3	2.148699304	0.44194229	0.584463953	1.090942883	12.45190032	0.001715895
C	-30.56776706	38.63604784	0.631881015	84.26444993	15.951633	0.000535025

**Table 8:** Statistical parameters of the linear regression model for  $DC_5(G)$

Property	c	m	r	SE	F	SF
BP	-9.9491118	33.71769041	0.861154364	58.28815287	68.87453	$1.63815 \times 10^{-8}$
MW	3.89270579	17.4087453	0.906683253	23.71794824	110.8879323	$1.77486 \times 10^{-10}$
CP	51.45428818	-1.77336066	-0.88193179	2.775726461	84.01259	$2.61856 \times 10^{-9}$
CT	249.091004	30.2827978	0.931218765	34.70892526	156.6799	$5.19221 \times 10^{-12}$
CV	56.85651629	49.91415613	0.896060247	72.41851184	97.78041	$6.11738 \times 10^{-10}$
XLogP3	0.442947795	0.399362027	0.869874211	0.663199766	74.63600475	$7.88384 \times 10^{-9}$
C	-151.9249024	32.90285986	0.886285773	50.35205299	87.88940145	$1.70745 \times 10^{-9}$

**Table 9:** Statistical parameters of the linear regression model for  $DC_6(G)$

Property	c	m	r	SE	F	SF
BP	180.5457264	4.652920387	0.906955938	48.29894449	111.2639	$1.71609 \times 10^{-10}$
MW	108.367961	2.298818773	0.913755988	22.84366602	121.4104864	$7.1552 \times 10^{-11}$
CP	40.72690449	-0.23273576	-0.88336143	2.759917976	85.2535	$2.27978 \times 10^{-9}$
CT	454.1142146	3.604983107	0.846050594	50.7693092	60.44805	$5.21148 \times 10^{-8}$
CV	348.3066195	6.728145065	0.921820162	63.23193123	135.7363	$2.29851 \times 10^{-11}$
XLogP3	2.690535178	0.055257473	0.918582329	0.531381019	129.6427695	$3.67739 \times 10^{-11}$
C	55.10305501	4.18299195	0.859932846	55.49103451	68.12503652	$1.80775 \times 10^{-8}$

**Table 7:** Statistical parameters of the linear regression model for  $DC_4(G)$ 

Property	c	m	r	SE	F	SF
BP	105.0029686	9.072267898	0.95780721	32.95543613	266.5381	$1.69293 \times 10^{-14}$
MW	69.10109023	4.532541884	0.975818384	12.29063196	478.3181878	$2.3329 \times 10^{-17}$
CP	44.71129672	-0.45911289	-0.94383583	1.945663389	195.8327	$4.87323 \times 10^{-13}$
CT	385.2817769	7.295577905	0.927373046	35.63052744	147.454	$9.77552 \times 10^{-12}$
CV	236.0824704	13.19587482	0.979243533	33.06427686	560.196	$3.79787 \times 10^{-18}$
XLogP3	1.799554835	0.107581805	0.968651515	0.334002089	364.8891577	$5.06614 \times 10^{-16}$
C	-20.20582819	8.347346375	0.929453383	40.11079566	152.319669	$6.9729 \times 10^{-12}$

**Table 10:** Statistical parameters of the linear regression model for  $DC_7(G)$ .

Property	c	m	r	SE	F	SF
BP	293.9299523	0.632584403	0.805527651	67.94444904	44.35169	$6.88863 \times 10^{-7}$
MW	164.0878855	0.313702247	0.814600246	32.61392775	47.33803159	$4.08253 \times 10^{-7}$
CP	34.87980785	-0.03095418	-0.76753113	3.774628204	34.40894	$4.74233 \times 10^{-6}$
CT	546.2088064	0.473501065	0.725964638	65.49523372	26.7426	$2.69467 \times 10^{-5}$
CV	510.5955432	0.921233505	0.824559476	92.29467826	50.97618	$2.22323 \times 10^{-7}$
XLogP3	3.9973906	0.007667701	0.832709683	0.744455458	54.2792695	$1.31363 \times 10^{-7}$
C	158.9852286	0.561070754	0.753523058	71.4743025	31.52946178	$8.84127 \times 10^{-6}$

### 3. Results and Discussion

To evaluate the effectiveness of the proposed degcity indices in predicting physicochemical properties of benzenoid hydrocarbons, linear regression analysis was carried out. The quality of each model is assessed using the correlation coefficient ( $r$ ), along with other statistical parameters.

#### 3.1. Performance of Degcity Indices

**First degcity index  $DC_1(G)$ :** The index  $DC_1(G)$  demonstrates good correlation with molecular weight (MW), critical volume (CV), and XLogP3. Its relationship with boiling point (BP) is moderate, while weaker correlations are observed with critical temperature (CT), critical pressure (CP), and molecular complexity (C).

**Second degcity index  $DC_2(G)$ :** The index  $DC_2(G)$  exhibits good predictive capability for CV and XLogP3, and moderate correlation with BP and MW. However, its performance with CT, CP, and C is comparatively less satisfactory.

**Third degcity index  $DC_3(G)$ :** Among all the indices,  $DC_3(G)$  shows relatively poor correlation with most of the considered physicochemical properties, indicating limited applicability in QSPR modeling for benzenoid hydrocarbons.

**Fourth degcity index  $DC_4(G)$ :** The index  $DC_4(G)$  provides the best overall performance. It shows excellent correlation with CV and MW, very strong correlation with BP and XLogP3, and good correlation with CT, CP, and C. This indicates that  $DC_4(G)$  is a reliable descriptor for predicting multiple properties. Compared with  $DC_5(G)$ , the index  $DC_4(G)$  gives relatively greater emphasis to eccentricity-related structural information through its square-root-based formulation. This enables  $DC_4(G)$  to simultaneously capture local connectivity patterns and the overall structural arrangement of benzenoid hydrocarbons, leading to stronger correlations with several physicochemical properties.

**Fifth degcity index  $DC_5(G)$ :** The index  $DC_5(G)$  exhibits good correlation with CT and moderate performance with MW. However, its predictive ability for other properties remains limited.

**Sixth degcity index  $DC_6(G)$ :** The index  $DC_6(G)$  shows moderate correlation with BP, MW, CV, and XLogP3, while weaker relationships are observed for CT, CP, and C.

**Seventh degcity index  $DC_7(G)$ :** The index  $DC_7(G)$  generally demonstrates moderate correlations across most properties, indicating average predictive capability.

#### 3.2. Comparison with Well-Known Topological Indices

The degcity indices are further compared with widely used topological indices such as Zagreb indices, Randić index, Harmonic index, Forgotten index, and others. As shown in Table 11, several degcity indices, particularly  $DC_1(G)$ ,  $DC_2(G)$ ,  $DC_4(G)$  and  $DC_6(G)$ , exhibit strong correlations with established descriptors.

**Table 11:** Correlation of degcity indices with well-known topological indices

Index	M <sub>1</sub>	M <sub>2</sub>	R	GA	H	F	SCI	FZE	SZE	ECI
DC <sub>1</sub>	0.9057	0.8777	0.9314	0.9025	0.9290	0.8892	0.9249	0.9645	0.9663	0.9991
DC <sub>2</sub>	0.8809	0.9743	0.9157	0.8799	0.9131	0.8607	0.9065	0.9743	0.9743	0.9990
DC <sub>3</sub>	0.7102	0.1081	0.6442	0.6883	0.6482	0.7380	0.6644	0.1081	0.1179	0.3249
DC <sub>4</sub>	0.9511	0.9200	0.9725	0.9473	0.9710	0.9368	0.9674	0.9200	0.9214	0.9870
DC <sub>5</sub>	0.9462	0.5191	0.9135	0.9309	0.9155	0.9574	0.9242	0.5191	0.5259	0.7016
DC <sub>6</sub>	0.8685	0.9756	0.9073	0.8686	0.9047	0.8465	0.8969	0.9756	0.9748	0.9964
DC <sub>7</sub>	0.7617	0.9999	0.8060	0.7626	0.8023	0.7372	0.7939	0.9999	0.9996	0.9702

### 3.3. Correlation among degcity indices

The interrelationships among the degcity indices are presented in Table 12. It can be observed that  $DC_1(G)$ ,  $DC_2(G)$  and  $DC_6(G)$  are highly correlated with one another, while  $DC_4(G)$  also shows strong association with these indices. In contrast,  $DC_3(G)$  exhibits relatively weak correlations with the others, suggesting that it captures different structural characteristics but with limited predictive strength.

**Table 12:** Correlation among degcity indices

Index	DC <sub>1</sub>	DC <sub>2</sub>	DC <sub>3</sub>	DC <sub>4</sub>	DC <sub>5</sub>	DC <sub>6</sub>	DC <sub>7</sub>
DC <sub>1</sub>	1						
DC <sub>2</sub>	0.996414	1					
DC <sub>3</sub>	0.353575	0.297225	1				
DC <sub>4</sub>	0.989178	0.983573	0.460100	1			
DC <sub>5</sub>	0.721468	0.682102	0.898567	0.801426	1		
DC <sub>6</sub>	0.992177	0.999136	0.273058	0.979017	0.664246	1	
DC <sub>7</sub>	0.963808	0.974067	0.103750	0.919220	0.515955	0.975655	1

### 3.4. Sensitivity

We can obtain more structural information if our topological indices have high sensitivity. Further details may be found in [9, 12]. The measure of sensitivity was introduced by E. V. Konstantinova [9], which is defined as

$$S = \frac{x-y}{x},$$

where  $x$  is the total number of nonisomorphic graphs considered (benzenoid hydrocarbons in our case) and  $y$  is the number of them that cannot be distinguished by the topological index. For Benzenoid hydrocarbons, degcity indices  $DC_2$ ,  $DC_4$ ,  $DC_5$ ,  $DC_6$  and  $DC_7$  display high sensitivity and  $DC_1$ ,  $DC_3$  show good sensitivity compared to other well-known topological indices as shown in Table 13.

**Table 13:** Sensitivity measures of different topological indices.

Index	Sensitivity
DC <sub>2</sub>	1.000000
DC <sub>4</sub>	1.000000
DC <sub>5</sub>	1.000000
DC <sub>6</sub>	1.000000
DC <sub>7</sub>	1.000000
DC <sub>1</sub>	0.961538
DC <sub>3</sub>	0.961538
FZE	0.961538
SZE	0.961538
ECI	0.961538
M <sub>2</sub>	0.769231
R	0.730769
GA	0.730769
SCI	0.730769
H	0.692308
AG	0.538462
M <sub>1</sub>	0.423077
F	0.423077

## 4. Conclusion

In this study, we investigated the applicability of degcity indices in the QSPR modeling of benzenoid hydrocarbons using linear regression analysis. The relationships between the proposed indices and several experimentally determined physicochemical properties, including boiling point, molecular weight, critical pressure, critical temperature, critical volume, XLogP3, and molecular complexity, were examined. The obtained results indicate that the degcity indices possess promising predictive capability, with varying levels of correlation performance. Among all the considered descriptors, the fourth degcity index  $DC_4(G)$  emerged as the most effective and consistent predictor, exhibiting strong correlations with multiple physicochemical properties. The indices  $DC_1(G)$ ,  $DC_2(G)$ , and  $DC_6(G)$  also demonstrated good predictive performance, while  $DC_3(G)$  showed comparatively weaker applicability in QSPR analysis.

The performance of  $DC_4(G)$  may be attributed to its balanced incorporation of degree and eccentricity information through a square-root-based formulation, which effectively captures both local connectivity and global structural characteristics of molecular graphs. In addition, the high sensitivity values obtained for several degcity indices confirm their strong discriminating ability for distinguishing benzenoid molecular structures.

Overall, the study suggests that degcity indices can serve as effective molecular descriptors in QSPR investigations of benzenoid hydrocarbons and related molecular systems. However, the present work is limited by the relatively small dataset size and the use of only simple linear regression models. External validation and cross-validation techniques were not considered in the current analysis. Future research may focus on larger datasets, advanced validation procedures, and machine learning-based predictive models to further assess and enhance the applicability of degcity indices in chemical informatics and QSPR modeling.

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