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A QSPR Study to Examine the Prediction Ability of Degcity Indices for Alkane Isomers

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Abstract:

In this article, a quantitative structure-property relationship (QSPR) method is used to examine the prediction ability of recently introduced degree-eccentricity based topological indices called degcity indices for 67 alkane isomers.

Mathematics Subject Classification (2020): 05C07, 05C12, 05C10, 05C09

Keywords: QSPR analysis, alkane isomers, topological indices, degcity indices.

1. Introduction:

Quantitative structure-property relationship (QSPR) and Quantitative structure- activity relationship have become a necessary tool to predict physicochemical proper ties of chemical compounds using topological indices [1, 2, 4, 5]. Further, prediction of these properties helps in minimizing the cost and time while designing a drug. QSPR is a mathematical model that describes the relationship between the chemical structure and its properties. Basically, regression based approaches are used when we have the numerical data of the chemical compounds. In this article, the linear regression model which is simple, transparent and easy to interpret, has been employed for the newly introduced degree-eccentricity based topological indices called degcity indices for physical properties of 67 alkane isomers. The degcity indices are defined as follows [6]:

$$DC_1(G) = \sum_{e=uv\in E(G)} [e_u + e_v]\,[d_u + d_v]$$

$$DC_2(G) = \sum_{e=uv\in E(G)} \frac{e_u + e_v}{d_u + d_v}$$

$$DC_3(G) = \sum_{e=uv\in E(G)} \frac{d_u + d_v}{e_u + e_v}$$

$$DC_4(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{e_u + e_v}{d_u + d_v}}$$

$$DC_5(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v}{e_u + e_v}}$$

$$DC_6(G) = \sum_{e=uv \in E(G)} \frac{e_u + e_v}{d_u d_v}$$

$$DC_7(G) = \sum_{e=uv \in E(G)} \frac{d_u + d_v}{e_u e_v}$$

here $e = uv$ is an edge, d_u, d_v represents the degree of the vertices u, v and e_u, e_u denote the eccentricity of the vertices u, v respectively of a graph $G = (V, E)$.

2. QSPR analysis of degcity indices for Alkane isomers

The experimental values of the physical properties [boiling points (bp), critical pressure (cp), critical temperature (ct), heats of vaporization (hv), melting points (mp), molar volume (mv), molar refraction (mr) and surface tensions (st)] for 67 alkane isomers is shown in Table 1 and are taken from [3]. The corresponding degcity indices of 67 alkane isomers are shown in Table 2.

Table 1: Experimental values of the physical properties of alkane isomers.

Alkanes	bp (°C)	cp (atm)	ct (°C)	hv (kJ)	mp (°C)	mv (cm^3)	mr (cm^3)	st (dyne/cm)
Butane	-0.5	37.47	152.01		-138.35			
2-methyl propane	-11.73	36	134.98		-159.6			
Pentane	36.074	33.31	196.62	26.42	-129.72	115.205	25.2656	16
2-methyl butane	27.852	32.9	187.7	24.59	-159.9	116.426	25.2923	15
2,2 dimethylpropane	9.503	31.57	160.6	21.78	-16.55	112.074	25.7243	
Hexane	68.74	29.92	234.7	31.55	-95.35	130.688	29.9066	18.42
2-methylpentane	60.271	29.95	224.9	29.86	-153.67	131.933	29.9459	17.38
3-methyalpentane	63.282	30.83	231.2	30.27	-118	129.717	29.8016	18.12
2,2-methylbutane	49.741	30.67	216.2	27.69	-99.87	132.744	29.9347	16.3
2,3-dimethylbutane	57.988	30.99	227.1	29.12	-128.54	130.24	29.8104	17.37
Heptanes	98.427	27.01	267.55	36.55	-90.61	146.54	34.5504	20.26
2-methylhexane	90.052	27.2	257.9	34.8	-118.28	147.656	34.5908	19.29
3-methylhexane	91.85	28.1	262.4	35.08	-119.4	145.821	34.4597	19.79
3-ethylpentane	93.475	28.6	267.6	35.22	-118.6	143.517	34.2827	20.44
2,2-dimethylpentane	79.197	28.4	247.7	32.43	-123.81	148.695	34.6166	18.02
2,3-dimethylpentane	89.784	29.2	264.6	34.24	-119.1	144.153	34.3237	19.96
2,4-dimethylpentane	80.5	27.4	247.1	32.88	-119.24	148.949	34.6192	18.15
3,3-dimethylpentane	86.064	30	263	33.02	-134.46	144.53	34.3323	19.59
Octane	125.665	24.64	296.2	41.48	-56.79	162.592	39.1922	21.76
2-methylheptane	117.647	24.8	288	39.68	-109.04	163.663	39.2316	20.6
3-methylheptane	118.925	25.6	292	39.83	-120.5	161.832	39.1001	21.17
4-methylheptane	117.709	25.6	290	39.67	-120.95	162.105	39.1174	21
3-ethylhexane	118.53	25.74	292	39.4		160.07	38.94	21.51
2,2-dimethylhexane	10.84	25.6	279	37.29	-121.18	164.28	39.25	19.6
2,3-dimethylhexane	115.607	26.6	293	38.79		160.39	38.98	20.99

2,4-dimethylhexane	109.42	25.8	282	37.76	-137.5	163.09	39.13	20.05
2,5-dimethylhexane	109.1	25	279	37.86	-91.2	164.69	39.25	19.73
3,3-dimethylhexane	111.96	27.2	290.84	37.93	-126.1	160.87	39	20.63
3,4-dimethylhexane	117.72	27.4	298	39.02		158.81	38.84	21.64
3-ethyl-2-methylpentane	115.65	27.4	295	38.52	-114.96	158.79	38.83	21.52
3-ethyl-3-methylpentane	118.25	28.9	305	37.99	-90.87	157.02	38.71	21.99
2,2,3-trimethylpentane	109.84	28.2	294	36.91	-112.27	159.52	38.92	20.67
2,2,4-trimethylpentane	99.23	25.5	271.15	35.13	-107.38	165.08	39.26	18.77
2,3,3-trimethylpentane	114.76	29	303	37.22	-100.7	157.29	38.76	21.56
2,3,4-trimethylpentane	113.46	27.6	295	37.61	-109.21	158.85	38.86	21.14
Nonane	150.79	22.74	322	46.44	-53.52	178.71	43.84	22.92
2-methyloctane	143.26	23.6	315	44.65	-80.4	179.77	43.87	21.88
3-methyloctane	144.18	23.7	318	44.75	-107.64	177.95	43.72	22.34
4-methyloctane	142.48	23.06	318.3	44.75	-113.2	178.15	43.76	22.34
3-ethylheptane	143	23.98	318	44.81	-114.9	176.41	43.64	22.81
4-ethylheptane	141.2	23.98	318.3	44.81		175.68	43.49	22.81
2,2-dimethylheptane	132.69	22.8	302	42.28	-113	180.5	43.91	20.8
2,3-dimethylheptane	140.5	23.79	315	43.79	-116	176.65	43.63	22.34
2,4-dimethylheptane	133.5	22.7	306	42.87		179.12	43.73	23.3
2,5-dimethylheptane	136	22.7	307.8	43.87		179.37	43.84	21.3
2,6- dimethylheptane	135.21	23.7	306	42.82	-102.9	180.91	43.92	20.83
3,3- dimethylheptane	137.3	24.19	314	42.66		176.897	43.687	22.01
3,4- dimethylheptane	140.6	24.77	322.7	43.84		175.349	43.5473	22.8
3,5- dimethylheptane	136	23.59	312.3	42.98		177.386	43.6379	21.77
4,4- dimethylheptane	135.2	24.18	317.8	42.66		176.897	43.6022	22.01
3-ethyl-2-methylhexane	138	24.77	322.7	43.84		175.445	43.655	22.8
4-ethyl-2-methylhexane	133.8	25.56	330.3	42.98		177.386	43.6472	21.77
3-ethyl-3-methylhexane	140.6	25.66	327.2	44.04		173.077	43.268	23.22
2,2,4- trimethylhexane	126.54	23.39	301	40.57	-120	179.22	43.7638	20.51
2,2,5- trimethylhexane	124.084	22.41	296.6	40.17	-105.78	181.346	43.9356	20.04
2,3,3- trimethylhexane	137.68	25.56	326.1	42.23	-116.8	173.78	43.4347	22.41
2,3,4- trimethylhexane	139	25.46	324.2	42.93		173.498	43.4917	22.8
2,3,5- trimethylhexane	131.34	23.49	309.4	41.42	-127.8	177.656	43.6474	21.27
3,3,4- trimethylhexane	140.46	26.45	330.6	42.28	-101.2	172.055	43.3407	23.27
3,3-diethylpentane	146.168	26.94	342.8	43.36	-33.11	170.185	43.1134	23.75
2,2-dimethyl-3-ethylpentane	133.83	25.96	322.6	42.02	-99.2	174.537	43.4571	22.38
2,3-dimethyl-3-ethylpentane	142	26.94	338.6	42.55		170.093	42.9542	23.87
2,4-dimethyl-3-ethylpentane	136.73	25.46	324.2	42.93	-122.2	173.804	43.4037	22.8

Table 2: Degcity indices for 67 alkane isomers.

Alkanes	DC_1	DC_2	DC_3	DC_4	DC_5	DC_6	DC_7
Butane	46	4.3333	2.2	3.5819	2.5492	6	5
2-methyl propane	36	2.25	4	2.5981	3.4641	3	1.5
Pentane	82	7.16666	2.4571	5.2911	3.0981	9.5	11
2-methyl butane	75	4.9666	3.45	4.4215	3.6815	6.5	5.8
2,2 dimethylpropane	60	2.4	6.6666	3.0984	5.1640	3	1.6
Hexane	134	11	2.4762	7.3346	3.4830	14	21.5833
2-methylpentane	122	8.0833	3.3714	6.2913	4.0609	10.25	12.7
3-methyalpentane	112	7.9166	3.6571	6.1731	4.2037	10.3333	11.9
2,2-methylbutane	114	5.3333	5.1	5.1075	4.9993	6.75	6.2666
2,3-dimethylbutane	104	5.6666	4.7	5.2886	4.8024	7.1111	6.6666
Heptane	194	15.3333	2.5772	9.4754	3.8896	19	36
2-methylhexane	186	12.15	3.1746	8.4629	4.3283	14.9166	24.3166
3-methylhexane	175	12.1	3.3571	8.3885	4.4246	15.25	23.5333
3-ethylpentane	138	10	4.2857	7.5825	4.9639	13	15.6
2,2-dimethylpentane	176	8.6166	4.5714	7.1081	5.1799	10.625	13.7
2,3-dimethylpentane	152	8.9166	4.5714	7.2042	5.1564	11.2222	13.7
2,4-dimethylpentane	162	9	4.2857	7.2915	5.0237	11	14.4
3,3-dimethylpentane	152	8.3333	5.2571	6.8808	5.5002	10.75	12.4
Octane	270	20.6666	2.5777	11.8942	4.2072	25	57
2-methylheptane	258	16.7166	3.1428	10.7188	4.6521	20.0833	40
3-methylheptane	246	16.7833	3.2756	10.6774	4.7242	20.6666	39.4
4-methylheptane	236	16.3833	3.4343	10.5190	4.8240	20.1666	37.8
3-ethylhexane	209	14.75	3.8333	9.9809	5.0911	18.5833	29.6
2,2-dimethylhexane	256	12.8166	4.0952	9.3847	5.3116	15.375	25.9166
2,3-dimethylhexane	227	13.3666	4.0555	9.5534	5.2612	16.3611	26.4666
2,4-dimethylhexane	227	13.25	4.0555	9.5168	5.2698	16.1666	26.2666
2,5-dimethylhexane	238	13.3	3.8730	9.5912	5.1735	15.8333	27.05
3,3-dimethylhexane	230	12.7166	4.5238	9.2335	5.5267	15.875	24.6333
3,4-dimethylhexane	216	13.3	4.2381	9.4763	5.3568	16.6666	25.6333
3-ethyl-2-methylpentane	178	11	5.2	8.6136	5.9166	13.8888	17.4
3-ethyl-3-methylpentane	178	10.5	5.8857	8.3212	6.2503	13.625	16.2
2,2,3-trimethylpentane	206	9.4976	5.7714	8.0403	6.2677	11.6666	14.7571
2,2,4-trimethylpentane	216	9.5333	5.4857	8.1083	6.1427	11.375	15.4
2,3,3-trimethylpentane	192	9.3809	6.1714	7.9313	6.4452	11.7083	14.2571
2,3,4-trimethylpentane	192	9.9166	5.4857	8.2353	6.1090	12.1111	15.5
Nonane	354	26.5	2.6315	14.3943	4.5432	31.5	83.3333
2-methyloctane	346	22.2833	3.0532	13.2430	4.9074	26.25	62.5
3-methyloctane	334	22.4166	3.1433	13.2190	4.9601	27	62
4-methyloctane	323	22.0666	3.2582	13.0865	5.03607	26.5833	60.2
3-ethylheptane	288	20	3.6594	12.4339	5.3251	24.6666	48.4

4-ethylheptane	270	19.0333	3.9105	12.1114	5.4906	23.5	43.8666
2,2-dimethylheptane	344	17.5166	3.8903	11.7350	5.5398	20.625	42.3333
2,3-dimethylheptane	310	18.3166	3.8412	11.9623	5.4792	22	43.7333
2,4-dimethylheptane	300	17.7666	4	11.7624	5.5865	21.25	41.8
2,5-dimethylheptane	310	18.1666	3.8412	11.9208	5.4867	21.75	43.4
2,6- dimethylheptane	322	18.1	3.7085	11.9623	5.4146	21.1666	44
3,3- dimethylheptane	316	17.6	4.1962	11.6407	5.7001	21.5	41.3333
3,4- dimethylheptane	288	17.95	4.1327	11.7575	5.6500	22.0277	41.4
3,5- dimethylheptane	298	18.2333	3.9740	11.8794	5.5588	22.3333	42.8
4,4- dimethylheptane	292	16.9666	4.5772	11.3564	5.9197	20.75	38.8
3-ethyl-2-methylhexane	261	16.0166	4.5317	11.1457	5.9278	19.6944	32.5333
4-ethyl-2-methylhexane	261	15.9	4.5317	11.1091	5.9363	19.5	32.3333
3-ethyl-3-methylhexane	264	15.4833	5	10.8625	6.1847	19.5	30.9
2,2,4- trimethylhexane	297	13.9166	4.9762	10.4386	6.2532	16.625	27.8666
2,2,5- trimethylhexane	308	13.9666	4.7936	10.5130	6.1568	16.2916	28.65
2,3,3- trimethylhexane	282	14.05	5.2222	10.4213	6.3569	17.0833	27.6809
2,3,4- trimethylhexane	268	14.5666	4.9365	10.6411	6.1935	17.7777	28.5666
2,3,5- trimethylhexane	279	14.5166	4.7539	10.6816	6.1064	17.2777	29.2
3,3,4- trimethylhexane	271	13.9738	5.4047	10.3425	6.4520	17.375	26.8190
3,3-diethylpentane	204	12.6666	6.5143	9.7616	7.0004	16.5	20
2,2-dimethyl-3-ethylpentane	232	11.5809	6.4	9.4498	7.0279	14.3333	18.4571
2,3-dimethyl-3-ethylpentane	218	11.5476	6.8	9.3717	7.1952	14.5833	18.0571
2,4-dimethyl-3-ethylpentane	218	12	6.1143	9.6447	6.8692	14.7777	19.2
2,2,3,3-tetramethylpentane	246	9.9916	7.3714	8.7806	7.5504	12.1875	15.35
2,2,3,4- tetramethylpentane	246	10.4976	6.6857	9.0714	7.2204	12.5555	16.5571
2,2,4,4- tetramethylpentane	270	10.0666	6.6857	8.9250	7.2618	11.75	16.4
2,3,3,4- tetramethylpentane	232	10.4285	7.0857	8.9818	7.3901	12.6666	16.1143

QSPR model

The following linear regression model has been considered in our study:

$$p = c + (TI)m, \qquad (2.1)$$

where p =physical property,

TI = topological index,

m = slope and

c = intercept.

From (2.1), we have the following linear regression models for each degcity index:

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

$$bp = 13.27901588 + [DC_1(G)]0.426959257$$

$$mv = 107.9731788 + [DC_1(G)]0.23539194$$

$$mr = 23.75622682 + [DC_1(G)]0.067847455$$

$$hv = 22.83965047 + [DC_1(G)]0.069105427$$

$ct = 175.0773391 + [DC_1(G)]0.495551823$

$cp = 35.31477462 - [DC_1(G)]0.03856781$

$st = 16.29686685 + [DC_1(G)]0.01996716$

$mp = -127.955158 + [DC_1(G)]0.088294707$

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

$bp = 31.04988349 + [DC_2(G)]5.93717183$

$mv = 124.407544 + [DC_2(G)]2.805200276$

$mr = 28.67589531 + [DC_2(G)]0.794970742$

$hv = 25.8381217 + [DC_2(G)]0.959212791$

$ct = 201.2256867 + [DC_2(G)]6.471266005$

$cp = 33.67457799 - [DC_2(G)]0.53365805$

$st = 17.31822025 + [DC_2(G)]0.266167235$

$mp = -126.82051 + [DC_2(G)]1.430158593$

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

$bp = 78.14183115 + [DC_3(G)]6.954556584$

$mv = 152.562511 + [DC_3(G)]2.133088993$

$mr = 34.96938081 + [DC_3(G)]0.9787904$

$hv = 38.1314234 + [DC_3(G)]0.137338076$

$ct = 233.8439648 + [DC_3(G)]11.7742465$

$cp = 26.86041045 - [DC_3(G)]0.04646359$

$st = 18.47857899 + [DC_3(G)]0.552335892$

$mp = -131.761505 + [DC_3(G)]5.050976546$

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

$bp = -16.4989001 + [DC_4(G)]13.45013711$

$mv = 96.71176846 + [DC_4(G)]6.864475862$

$mr = 20.44086971 + [DC_4(G)]1.985844976$

$hv = 17.63324615 + [DC_4(G)]2.2145359$

$ct = 143.2326772 + [DC_4(G)]15.32012665$

$cp = 37.42256384 - [DC_4(G)]1.15266731$

$st = 14.40690151 + [DC_4(G)]0.678716152$

$mp = -134.702638 + [DC_4(G)]2.874717567$

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

$bp = -20.6966854 + [DC_5(G)]23.89119843$

$mv = 101.6872049 + [DC_5(G)]10.97580627$

$mr = 19.4777125 + [DC_5(G)]3.611225515$

$hv = 23.75221549 + [DC_5(G)]2.721724336$

$ct = 112.6696821 + [DC_5(G)]31.9559166$

$cp = 34.51347011 - [DC_5(G)]1.44608312$

$st = 13.94876885 + [DC_5(G)]1.268777228$

$mp = -145.121389 + [DC_5(G)]6.728758796$

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

$bp = 27.69356941 + [DC_6(G)]5.050859056$

$mv = 123.7363545 + [DC_6(G)]2.330814221$

$mr = 28.43546606 + [DC_6(G)]0.663579393$

$hv = 25.31842795 + [DC_6(G)]0.814600271$

$ct = 197.3989787 + [DC_6(G)]5.515666646$

$cp = 33.8062625 - [DC_6(G)]0.44345377$

$st = 17.08117271 + [DC_6(G)]0.23150087$

$mp = -127.425425 + [DC_6(G)]1.207724891$

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

$bp = 67.27596199 + [DC_7(G)]1.529070868$

$mv = 142.1419746 + [DC_7(G)]0.711670274$

$mr = 33.82487071 + [DC_7(G)]0.197303842$

$hv = 31.77380227 + [DC_7(G)]0.247913936$

$ct = 242.921077 + [DC_7(G)]1.585935701$

$cp = 30.68731308 - [DC_7(G)]0.14725419$

$st = 19.16890438 + [DC_7(G)]0.062273199$

$mp = -120.654029 + [DC_7(G)]0.452116951$

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 3, 4, 5, 6, 7, 8 and 9 respectively, where N denotes the number of alkane isomers taken into consideration and r represents the correlation coefficient.

Table 3: DC_1 - Statistical parameters.

Property	N	c	m	R
bp	67	13.27901588	0.426959257	0.838000936
mv	67	107.9731788	0.23539194	0.938412894
mr	65	23.75622682	0.067847455	0.909490534
hv	65	22.83965047	0.069105427	0.903714337
ct	67	175.0773391	0.495551823	0.836686514
cp	67	35.31477462	-0.03856781	-0.94911677
st	64	16.29686685	0.01996716	0.693357879
mp	52	-127.955158	0.088294707	0.267361407

Table 4: DC_2 - Statistical parameters.

Property	N	c	m	R
bp	67	31.04988349	5.93717183	0.748665265
mv	67	124.407544	2.805200276	0.740806029
mr	65	28.67589531	0.794970742	0.705917627
hv	65	25.8381217	0.959212791	0.830944912
ct	67	201.2256867	6.471266005	0.701960927
cp	67	33.67457799	-0.53365805	-0.84373814
st	64	17.31822025	0.266167235	0.613419089
mp	52	-126.82051	1.430158593	0.276652503

Table 5: DC_3 - Statistical parameters.

Property	N	c	m	r
bp	67	78.14183115	6.954556584	0.220619876
mv	67	152.562511	2.133088993	0.147440272
mr	65	34.96938081	0.9787904	0.227488316
hv	65	38.1314234	0.137338076	0.031139723
ct	67	233.8439648	11.7742465	0.321309773
cp	67	26.86041045	-0.04646359	-0.01848096
st	64	18.47857899	0.552335892	0.340163655
mp	52	-131.761505	5.050976546	0.254716598

Table 6: DC_4 – Statistical Parameters.

Property	N	c	m	r
bp	67	-16.4989001	13.45013711	0.862614638
mv	67	96.71176846	6.864475862	0.885290666
mr	65	20.44086971	1.985844976	0.861164447
hv	65	17.63324615	2.2145359	0.936866834
ct	67	143.2326772	15.32012665	0.845216737
cp	67	37.42256384	-1.15266731	-0.92689521
st	64	14.40690151	0.678716152	0.748316009
mp	52	-134.702638	2.874717567	0.280848088

Table 7: DC_5 - Statistical parameters.

Property	N	c	m	r
bp	67	-20.6966854	23.89119843	0.637771448
mv	67	101.6872049	10.97580627	0.596519561
mr	65	19.4777125	3.611225515	0.659941004
hv	65	23.75221549	2.721724336	0.485231548
ct	67	112.6696821	31.9559166	0.733827591
cp	67	34.51347011	-1.44608312	-0.48401291
st	64	13.94876885	1.268777228	0.629373046
mp	52	-145.121389	6.728758796	0.285250381

Table 8: DC_6 - Statistical parameters.

Property	N	c	m	r
bp	67	27.69356941	5.050859056	0.750025513
mv	67	123.7363545	2.330814221	0.72446767
mr	65	28.43546606	0.663579393	0.693531971
hv	65	25.31842795	0.814600271	0.830562917
ct	67	197.3989787	5.515666646	0.704570439
cp	67	33.8062625	-0.44345377	-0.82564944
st	64	17.08117271	0.23150087	0.625730723
mp	52	-127.425425	1.207724891	0.273572458

Table 9: DC_7 - Statistical parameters.

Property	N	c	m	r
bp	67	67.27596199	1.529070868	0.629932386
mv	67	142.1419746	0.711670274	0.633122823
mr	65	33.82487071	0.197303842	0.5902105
hv	65	31.77380227	0.247913936	0.723480317
ct	67	242.921077	1.585935701	0.562040381
cp	67	30.68731308	-0.14725419	-0.7606249
st	64	19.16890438	0.062273199	0.494779888
mp	52	-120.654029	0.452116951	0.291104999

3. Results and concluding remarks

We adopt the following scale given by M. Randic [4], to examine the prediction ability of degcity indices:

Correlation coefficient ($\|r\|$)	Quality
0.990 (and higher)	Outstanding
0.975 (and higher)	Excellent
0.950 (and higher)	Very good
0.925 (and higher)	Good
0.900 (and higher)	Fair
0.800 (and higher)	Mediocre
Below 0.800	Uninteresting
Below 0.100	Non-existent

From the Table-3, 4, 5, 6, 7, 8, 9, we observe that the values of the correlation coefficient (r) for the physical properties of 67 alkane isomers with the first degcity index $DC_1(G)$ are found to be good with *mv*, *cp* and it is fair with *mr*, *hv*. Whereas the correlation is good with *hv, cp* and mediocre with *bp, mv, mr, ct* for the fourth degcity index $DC_4(G)$. Also the second degcity index

$DC_2(G)$ and sixth degcity index $DC_6(G)$ are mediocre with *hv, cp* and uninteresting for other physical proper- ties. Further, the remaining degcity indices $DC_3(G)$, $DC_5(G)$, $DC_7(G)$ doesn't show correlation since the correlation coefficient is less than 0.800.

Finally, in this QSPR study we conclude that among all degcity indices, $DC_1(G)$ and $DC_4(G)$ show good prediction ability with some physical properties of 67 alkane isomers.

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