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On the Acharya Index for Characterization of Chemical Graphs

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Abstract
Recently Shirkol et. al [7], have put forward a novel topological descriptor namely the Acharya Index of a molecular graph G in honor of Late. Prof. B. D. Acharya. In this paper, we carry out quantitative structure property analysis of 74 alkanes using the Acharya index. Further, we compare these results with the Wiener and terminal Wiener indices. Our study reveals some interesting results based on the predicting power of these topological descriptors.

Keywords: Wiener index, Terminal Wiener Index, Acharya Index,QSPR analysis

Subject Classification: Mathematics subject classification *05C90, 05C35, 05C12.*

1.Introduction and Main Result

The molecular descriptor is logic and mathematical procedure which transform chemical information encoded within a symbolic representation of a molecule into a useful member or the result of some standardized experiments. Chemical graph theory is the branch of mathematical chemistry where in chemical graphs are called molecular graphs. Molecular graph is a simple carbon atom -skeleton of an organic molecule (hydrocarbons). Thus vertices of molecular graph represent the carbon atoms and its edges represent the carbon-carbon bonds. Hence the chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. Topological indices are convenient means of translating chemical constitution into numerical values which can be used for correlation with physical properties in quantitative structure-property/activity relationship (QSPR/QSAR) studies. The use of graph invariant (topological indices) in QSPR and QSAR studies has become one of the major interests in recent years.
The oldest structural descriptor was defined in 1947 by H. Wiener [1]. This index is known as Wiener index. It is defined as sum of distances between all pair of vertices of graph

$$W = W(G) = \sum_{(u,v)\subseteq V(G)} d_G(u,v)$$

The Terminal Wiener index of a graph [2] is defined as the sum of the distances between all the pairs of pendant vertices.

$$TW = TW(G) = \sum_{1<i<j<k} d(v_i, v_j / G)$$

Details on chemical application and mathematical properties of Wiener index and terminal Wiener index and other degree and distance based topological indices see the reviews and references quoted therein [3, 4, 5, 6,10-32].

Shirkol et.al have defined novel topological index viz. Acharya index $AI_\lambda(G)$ of a graph *G* [7] as the sum of distances between all pairs of degree d vertices i.e.

$$AI_\lambda(G) = \sum_{\substack{1\le d\le n-1 \\ 1\le i\le p}} \mu(d,i)\cdot i$$

where $\mu(d,i)$ denotes pair of degree d vertices at distance *i*, *p*=diam(*G*)

Acharya Polynomial *AP* (*G*,*i*) is defined as follows

$$AP(G,i) = \sum_{\substack{1\le d\le n-1 \\ 1\le i\le p}} \mu(d,i)\cdot x^i$$

The following relationship between Acharya index and Acharya Polynomial is noted in [7,8 ,9]

$AI_\lambda(G) = AP^1(G,i)$

It is noted that $W(G) \ge AI_\lambda(G) \ge TW(G)$ and $W(G) = AI_\lambda(G)$ if *G* is a regular graph and $AI_\lambda(G) = TW(G)$ if *G* is a star graph.

1. The use of Acharya index in the QSPR studies

We have used the Acharya index and its variants for modeling eight representatives physical properties (boiling points (bp), molar volumes (mv) at 20, molar refractions (mr) at 20, heats of vaporization (hv) at 25, critical temperature (ct), critical pressure (cp) surface tensions (st) 20 and melting points (mp)) of the 74 alkanes from ethane to nonanes. The value of Wiener index, Acharya index and terminal Wiener index are listed in Table 1.

2. Regression Models

We have tested the following linear regression model

P=A+B(TI)

where P=physical property, TI=topological index.

We have obtained the following linear models for Wiener index, Acharya index and Terminal Wiener index

1. **Wiener index *W*** (*G*):

bp=4.249+[W (G)] 1.425
mv=113.9+[W (G)]0:643
mr=24.83+[W (G)]0.193
hv=24.34+[W (G)]0.183
ct=159.3+[W (G)]1.696
cp=36.15+[W (G)](-.126)
st=16.12+[W (G)].063
mp=-135.1+[W (G)].369

Table1

Sl.No	ALKANES	W	AI	TW	Bp(oC)	mv(cm3)	mr(cm3)	hv(kJ)	ct(oC)	cp(atm)	st(dyne/cm)	mp(oC)
1	ethane	1	1	1	-88.63				32.27	48.2		-183.27
2	propane	4	2	2	-42.07				96.8	42.01		-187.69
3	butane	10	4	3	-0.5				152.01	37.47		-138.35
4	2-methylpropane	9	6	6	-11.73				134.98	36		-159.6
5	pentane	20	8	8	36.074	115.205	25.2656	26.42	196.62	33.31	16	-129.72
6	2-methylbutane	18	8	8	27.852	116.426	25.2923	24.59	187.7	32.9	15	-159.9
7	2,2-dimethylpropane	16	12	8	9.503	122.074	25.7243	21.78	160.6	31.57		-16.55
8	hexane	35	15	5	68.74	130.688	29.9066	31.55	234.7	29.92	18.42	-95.35
9	2-methylpentane	32	11	10	60.271	131.933	29.9459	29.86	224.9	29.95	17.38	-153.67
10	3-methylpentane	31	12	10	63.282	129.717	29.8016	30.27	231.2	30.83	18.12	-118
11	2,2-methylbutane	28	15	15	49.741	132.744	29.9347	27.69	216.2	30.67	16.3	-99.87
12	2,3-methylbutane	29	17	16	57.988	130.24	29.8104	29.12	227.1	30.99	17.37	-128.54
13	heptane	56	26	6	98.427	146.54	34.5504	36.55	267.55	27.01	20.26	-90.61
14	2-methylhexane	52	16	12	90.052	147.656	34.5908	34.8	257.9	27.2	19.29	-118.28
15	3-methylhexane	50	18	12	91.85	145.821	34.4597	35.08	262.4	28.1	19.79	-119.4
16	3-ethylpentane	48	18	12	93.475	143.517	34.2827	35.22	267.6	28.6	20.44	-118.6
17	2,2-methylpentane	46	19	16	79.197	148.695	34.6166	32.43	247.7	28.4	18.02	-123.81
18	2,3-methylpentane	46	20	15	89.784	144.153	34.3237	34.24	264.6	29.2	19.96	-119.1
19	2,4-methylpentane	48	22	16	80.5	148.949	34.6192	32.88	247.1	27.4	18.15	-119.24
20	3,3-methylpentane	44	20	14	86.064	144.53	34.3323	33.02	263	30	19.59	-134.46
21	2,2,3-trimethylbutane	42	26	26	80.882	145.191	34.3736	32.04	258.3	29.75	18.76	-24.91
22	octane	84	42	7	125.665	162.592	39.1922	41.48	296.2	24.64	21.76	-56.79
23	2-methylheptane	79	24	14	117.647	163.663	39.2316	39.68	288	24.8	20.6	-109.04
24	3-methylheptane	76	27	14	118.925	161.832	39.1001	39.83	292	25.6	21.17	-120.5
25	4-methylheptane	75	28	14	117.709	162.105	39.1174	39.67	290	25.6	21	-120.95
26	3-ethylhexane	72	27	14	118.534	160.072	38.9441	39.4	292	25.74	21.51	
27	2,2-dimethylhexane	71	25	21	106.84	164.285	39.2525	37.29	279	25.6	19.6	-121.18
28	2,3-dimethylhexane	70	24	22	115.607	160.395	38.9808	38.79	293	26.6	20.99	
29	2,4-dimethylhexane	71	27	23	109.429	163.093	39.13	37.76	282	25.8	20.05	-137.5
30	2,5-dimethylhexane	74	28	24	109.103	164.697	39.2596	37.86	279	25	19.73	-91.2
31	3,3-dimethylhexane	67	27	21	111.969	160.879	39.0087	37.93	290.84	27.2	20.63	-126.1
32	3,4-dimethylhexane	68	26	22	117.725	158.814	38.8453	39.02	298	27.4	21.64	
33	3-ethyl-2-methylpentane	67	25	22	115.65	158.794	38.8362	38.52	295	27.4	21.52	-114.96
34	3-ethyl-3-methylpentane	64	27	21	118.259	157.026	38.7171	37.99	305	28.9	21.99	-90.87
35	2,2,3-trimethylpentane	63	30	27	109.841	159.526	38.9249	36.91	294	28.2	20.67	-112.27
36	2,2,4-trimethylpentane	66	32	32	99.238	165.083	39.2617	35.13	271.15	25.5	18.77	-107.38
37	2,3,3-trimethylpentane	62	30	27	114.76	157.292	38.7617	37.22	303	29	21.56	-100.7
38	2,3,4-trimethylpentane	65	36	32	113.467	158.852	38.8681	37.61	295	27.6	21.14	-109.21
39	2,2,3,3-trimethylbutane	58	41	40	106.47				270.8	24.5		
40	nonane	120	64	8	150.798	178.713	43.8423	46.44	322	22.74	22.92	-53.52
41	2-methyllocactane	114	36	16	143.26	179.773	43.8795	44.65	315	23.6	21.88	-80.4
42	3-methyllocactane	110	40	16	144.18	177.952	43.7296	44.75	318	23.7	22.34	-107.64
43	4-methyllocactane	108	42	16	142.48	178.15	43.7687	44.75	318.3	23.06	22.34	-113.2
44	2-ethylheptane	104	40	16	143	176.41	43.642	44.81	318	23.98	22.81	-114.9
45	4-ethylheptane	102	40	16	141.2	175.685	43.4907	44.81	318.3	23.98	22.81	
46	2,2-dimethylheptane	104	34	24	132.69	180.507	43.9138	42.28	302	22.8	20.8	-113
47	2,3-dimethylheptane	102	30	25	140.5	176.653	43.6369	43.79	315	23.79	22.34	-116
48	2,4-dimethylheptane	102	38	26	133.5	179.12	43.7393	42.87	306	22.7	23.3	
49	2,5-dimethylheptane	104	36	27	136	179.371	43.8484	43.87	307.8	22.7	21.3	

50	2,6-dimethylheptane	108	35	28	135.21	180.914	43.9258	42.82	306	23.7	20.83	-102.9
51	3,3-dimethylheptane	98	37	24	137.3	176.897	43.687	42.66	314	24.19	22.01	
52	3,4-dimethylheptane	98	34	25	140.6	175.349	43.5473	43.84	322.7	24.77	22.8	
53	3,5-dimethylheptane	100	36	26	136	177.386	43.6378	42.98	312.3	23.59	21.77	
54	4,4-dimethylheptane	96	38	24	135.2	176.897	43.6022	42.66	317.8	24.18	22.01	
55	3-ethyl-2-methylhexane	96	32	25	138	175.445	43.655	43.84	322.7	24.77	22.8	
56	4-ethyl-2-methylhexane	98	34	26	133.8	177.386	43.6472	42.98	330.3	25.56	21.77	
57	3-ethyl-3-methylhexane	92	37	24	140.6	173.077	43.268	43.04	327.2	25.66	23.22	
58	3-ethyl-4-methylhexane	94	29	25	140.4	172.844	43.3746	43.95	312.3	23.59	23.27	
59	2,2,3-trimethylhexane	92	35	34	133.6	175.878	43.6226	41.91	318.1	25.07	21.86	
60	2,2,4-trimethylhexane	94	38	36	126.54	179.22	43.7638	0.57	301	23.39	20.51	-120
61	2,2,5-trimethylhexane	98	39	38	124.084	181.346	43.9356	40.17	296.6	22.41	20.04	-105.78
62	2,3,3-trimethylhexane	90	22	32	137.68	173.78	43.4347	42.23	326.1	25.56	22.41	-116.8
63	2,3,4-trimethylhexane	92	40	36	139	173.498	43.4917	42.93	324.2	25.46	22.8	
64	2,3,5-trimethylhexane	96	44	38	131.34	177.656	43.6474	41.92	309.4	23.49	21.27	-127.8
65	2,4,4-trimethylhexane	92	38	36	130.648	177.187	43.6598	40.84	309.1	23.79	21.17	-133.38
66	3,3,4-trimethylhexane	88	37	34	140.46	172.055	43.3407	42.28	330.6	26.45	23.27	-101.2
67	3,3-diethylpentane	88	36	24	146.168	170.185	43.1134	43.36	342.8	26.94	23.75	-33.11
68	2,2-dimethyl-3-ethylpentane	88	36	32	133.83	174.537	43.4571	42.02	322.6	25.96	22.38	-99.2
69	2,3-dimethyl-3-ethylpentane	86	36	34	142	170.093	42.9542	42.55	338.6	26.94	23.87	
70	2,4-dimethyl-3-ethylpentane	90	40	36	136.73	173.804	43.4037	42.93	324.2	25.46	22.8	-122.2
71	2,2,3,3-tetramethylpentane	82	47	44	140.274	169.495	43.2147	41	334.5	27.04	23.38	-99
72	2,2,3,4-tetramethylpentane	86	48	47	133.016	173.557	43.4359	41	319.6	25.66	21.98	-121.09
73	2,2,4,4-tetramethylpentane	88	50	40	122.284	178.256	43.8747	38.1	301.6	24.58	20.37	-66.54
74	2,3,3,4-tetramethylpentane	84	48	47	141.551	169.928	43.2016	41.75	334.5	26.85	23.31	-102.12

2. **Acharya index** $AI_{\lambda}(G)$:

bp=13.78+[$AI_{\lambda}(G)$]3.76

mv=121.7+[$AI_{\lambda}(G)$]1.333

mr=26.92+[$AI_{\lambda}(G)$]0.41

hv=27.13+[$AI_{\lambda}(G)$].361

ct=168.6+[$AI_{\lambda}(G)$]3.829

cp=35.12+[$AI_{\lambda}(G)$](-.275)

st=16.79+[$AI_{\lambda}(G)$].134

mp=-141.8+[TW (G)]1.121

3. **Terminal Wiener index** *TW* (*G*):

bp=49.58+[TW (G)] 2.589

mv=139.1 [TW (G)] 1.029

mr=31.95[TW (G)] 0.331

hv=34.43+[TW (G)] 0.166

ct=207.1+[TW (G)] 3.359

cp=31.68+[TW (G)] (-.21)
st=18.91+[TW (G)] 0.089
mp=-121.3+[TW (G)] 0.511

Table 2. Stastical parameter for the linear QSPR model for Wiener index

Physical Property	N	a	b	r	s	f
Boiling point	74	4.249	1.425	0.917	11.9596	381
Molar volume	69	113.9	0.643	0.972	6.1736	1.15
Molar refraction	69	24.83	0.193	0.962	7.2104	822
Heats of vaporization	69	24.34	0.183	0.676	19.3619	56.2
Critical temperature	74	159.3	1.696	0.883	14.08484	255
Critical Pressure	74	36.15	-0.126	0.873	14.648	230
Surface Tension	68	16.12	0.063	0.818	14.6207	133
Melting point	56	135.1	0.369	0.361	29.4181	8.08

Table 3. Stastical parameter for the linear QSPR model for Acharya index

Physical Property	N	a	b	r	s	f
Boiling point	74	13.78	3.16	0.839	6.7353	171
Molar volume	69	121.7	1.333	0.841	5.93479	161
Molar refraction	69	26.92	0.41	0.849	5.78436	173
Heats of vaporization	69	27.13	0.361	0.556	9.10618	30
Critical temperature	74	168.6	3.829	0.822	7.01499	150
Critical Pressure	74	35.12	-0.275	0.78	7.74217	112
Surface Tension	68	16.79	0.134	0.742	7.24129	80.7
Melting point	56	-141.8	1.121	0.472	11.9868	15.5

Table 4. Stastical parameter for the linear QSPR model for Terminal Wiener index

Physical Property	N	a	b	r	s	f
Boiling point	74	49.58	2.589	0.623	8.77462	45.6
Molar volume	69	139.1	1.029	0.616	8.18614	40.9
Molar refraction	69	31.95	0.336	0.65	7.89562	49
Heats of vaporization	69	34.43	0.166	0.242	10.0805	4.17
Critical temperature	74	207.1	3.359	0.654	8.48711	53.7
Critical Pressure	74	31.68	-0.21	0.542	9.42745	29.9
Surface Tension	68	18.91	0.089	0.469	9.10088	18.8
Melting point	56	-121.3	0.511	0.192	11.88869	2.06

4. Discussion and Concluding Remarks

By the observation in the Table 2, Table3 and Table 4 as a result of QSRP analysis, it is possible to draw number conclusions for the topological indices.

First, the well-known and much studied Wiener index, is a more suitable tool to predict physical properties of alkanes. Especially Boiling point(Bp), Molar volume (mv), Molar refraction(mr), Critical

temperature(ct),Critical pressure(cp) and Surface tension(st) of alkanes with correlation coefficient r=0.917, 0.972,0.962, 0.883, 0.873 and 0.818 respectively.

Motivated by Terminal Wiener index Shirkol et. al have defined a new topological Acharya index. The QSRP analysis of Acharya index was correlated with each of these physical properties and surprisingly, we can see that the Acharya index shows good correlation with boiling points (bp), molar volume (mv) and molar refraction (mr) with correlation coefficient value 0.839, 0.841 and 0.849 respectively.

By the observation in Table 4, one can say that the terminal Wiener index has less predictive ability. The correlation coefficient value 0.192 to 0.654.However all three topological indices weaker correlation to Heats of vaporization (hv) and Melting point (mp)And it shows good correlation with all physical properties of alkanes comparing with Terminal Wiener index. From a practical point of view, the topological indices for which the absolute value of correlation coefficient less than.8 can be characterized as useless. Thus Acharya index can be considered for study of physical properties of chemical compounds.

5. Correlation between Acharya index, terminal Wiener index with physical properties 74 alkanes.

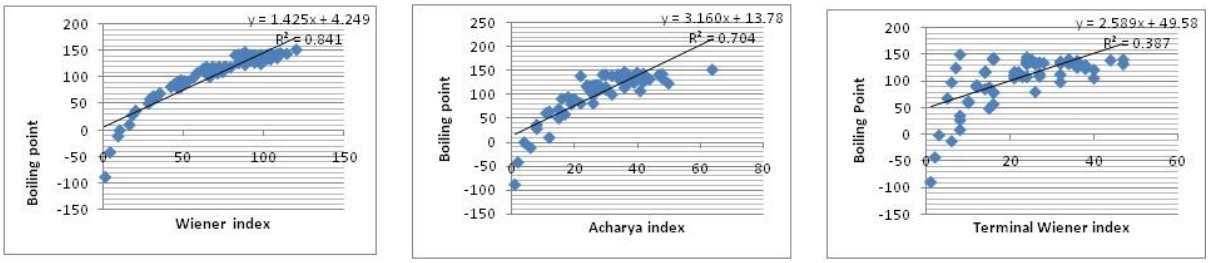

Figure1: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (Bp) of 74 alkanes.

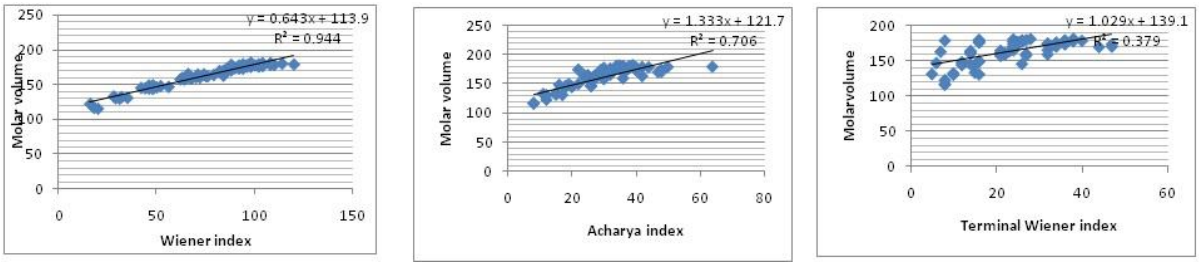

Figure2: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (mv) of 74 alkanes.

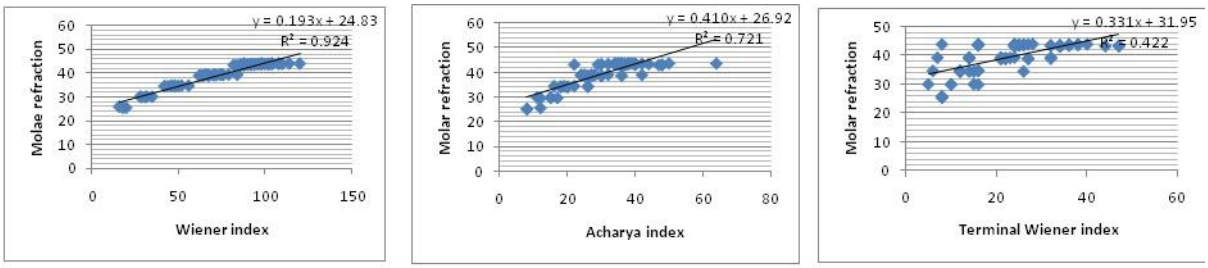

Figure3: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (mr) of 74 alkanes.

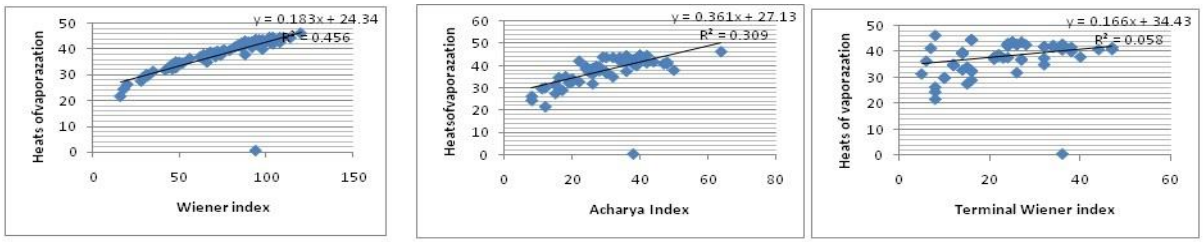

Figure4: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (hv) of 74 alkanes.

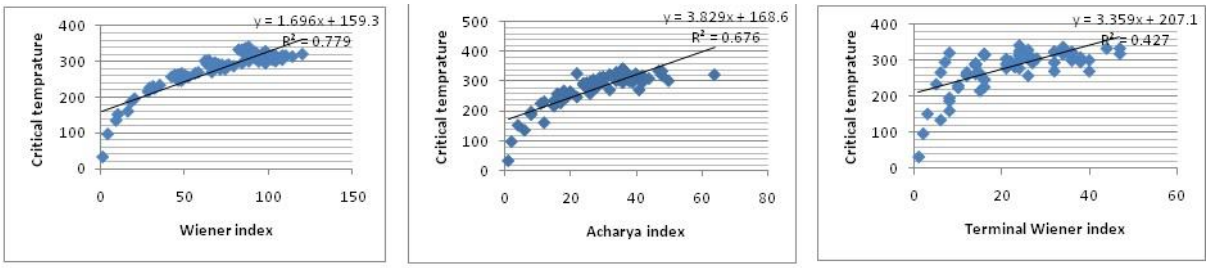

Figure5: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (ct) of 74 alkanes.

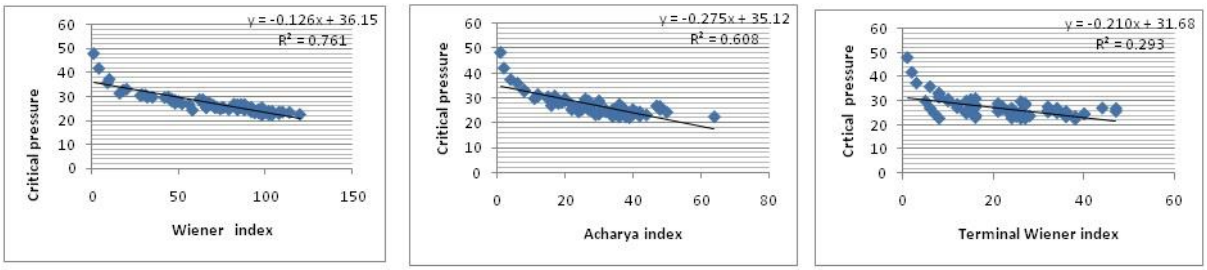

Figure6: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (cp) of 74 alkanes.

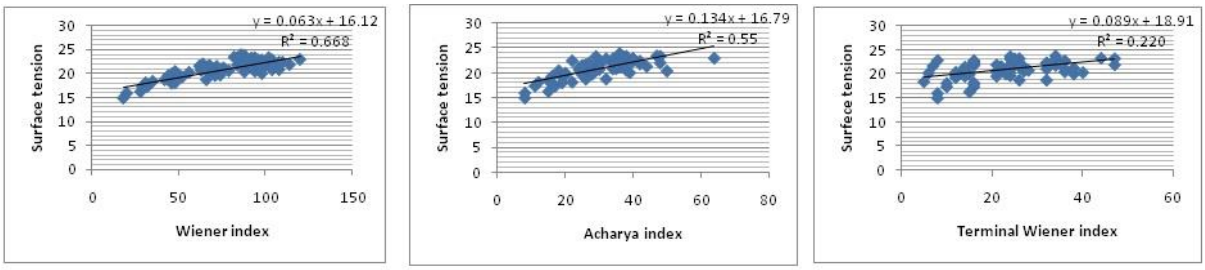

Figure7: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (st) of 74 alkanes.

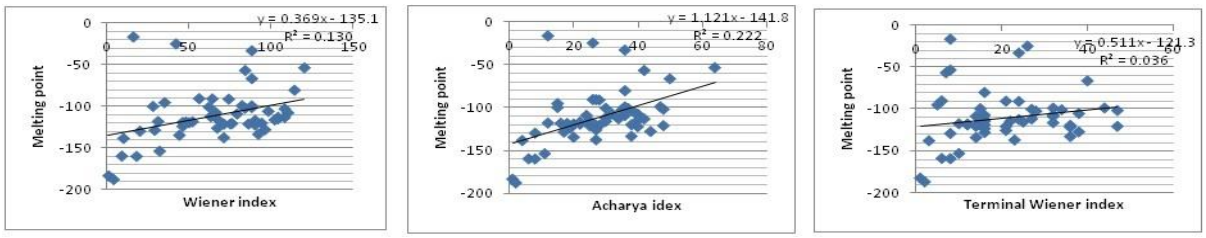

Figure8: Correlation between Wiener index, Acharya index and terminal Wiener index with physical properties (mp) of 74 alkanes.

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