Section A-Research paper

Quantitative Structure Property Relationship Analysis of Kulli's Topological Indices

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Abstract:

Molecular descriptor is a number associated with the moleculargraph.Theapplications of molecular descriptors in predicting the physico-chemico properties of chemical compounds framed a remarkable benchmark in the field of mathematical chemistry. In this paper, we consider Kulli's molecular descriptors to examine their applications in QSPR(Quantitative Structure Property Relationship) study ofalkanes.TheresultsofQSPR-analysisdemonstratedF-Somborindex(FSLI),sumconnectivity Gourava index(SCGI), product connectivity Gourava index(PCGI), multiplicative atom bond sum connectivity index(MASCI) and Revan Sombor index(RSI) shows good correlation with the physical properties of alkanes.

Keywords: F-Sombor index, multiplicative atom bond sum connectivity index, QSPR

***AMS* Subject Classification:** 05C90; 05C12.

1. Introduction

A graph is said to be simple if it doesn't contain multiple edges or loops. Throughoutthispapersimpleandundirectedgraphsareconsideredwithvertexset$V$andedgeset$E$.T he order and size of $G$is denoted by $|V| = n$and $|E| = m$respectively. The degree of avertex $v \in V$is the number of edges incident to $v$and it is denoted by$d_G(v)$. The degreeof an edge $e = uv$is defined as $d_G(e) = d_G(u) + d_G(v) - 2$. For undefined terminology in this paper refer[3].

Topological index is simply a numerical associated with the molecular graph. So far, large number of such quantities are put forward by many researchers right from 1972.

One of the most useful topological indices are the Zagreb indices [2] which are defined as:

$$M_1(G) = \sum_{i=1}^{n} d_G(v)^2 ,$$

$$M_2(G) = \sum_{u,v \in E(G)} d_G(u)\, d_G(v) ,$$

Where $M_1$and M_2 are the first and second Zagreb indices respectively.

Motivated by degree based topological indices, Kulli[4- 0] put forward the following topological indices:

Table 1: Molecular Descriptors

SI. No.	Molecular descriptor	Abbreviation	Definition
1	F-Sombor Index [6]	FSLI	$\sum_{uv \in E(G)} \sqrt{(d(u)^4 + d(v)^4)}$
2	Sum Connectivity Gourava Index [9]	SCGI	$\sum_{uv \in E(G)} \frac{1}{\sqrt{(d(u)+d(v)) + (d(u)*d(v))}}$
3	Product Connectivity Gourava Index [11]	PCGI	$\sum_{uv \in E(G)} \frac{1}{\sqrt{(d(u)+d(v)) * (d(u)*d(v))}}$
4	Multiplicative Atom Bond Sum Connectivity Index [8]	MASCI	$\sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$
5	Sum Augmented Index [10]	SAI	$\sum_{uv \in E(G)} \left(\frac{d(u)+d(v)}{d(u)+d(v)-2} \right)^3$
6	Revan Sombor Index [4]	RSI	$\sum_{uv \in E(G)} \sqrt{(\Delta(G)+\delta(G)-d(u))^2 + (\Delta(G)+\delta(G)-d(v))^2}$

2. Applications of Kulli's Molecular Descriptors

Here we consider the topological indices depicted in Table1 along with eight representative physical properties [boiling points(BP), molar volumes(mv) at 20°C, molar refractions(mr) at 20°C, heats of vaporization(hv) at 25°C, surface tensions(st) 20°C and melting points (mp)] of the 67 alkanes from n-butanes to nonanes. Values for this property were taken from[11]. The above said distance-based topological indices and the experimental values for the physical properties of 67 alkanes are listed in Table2.

Table 2. Physical Properties of alkanes

Sl. No.	**Alkane**	**bp** (^0C)	**mv** (cm^3)	**mr** (cm^3)	**hv (kJ)**	**ct** (^0C)	**cp(atm)**	**st(dyne/cm)**	**mp** (^0C)
1	Butane	-0.500				152.01	37.47		-138.35
2	2-methyl propane	-11.730				134.98	36		-159.60
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00	-129.72
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00	-159.90
5	2,2 dimethylpropane	9.503	112.074	25.7243	21.78	160.60	31.57		-16.55
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42	-95.35
7	2-methylhexane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
8	3-methylhexane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.28
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
10	2,3-dimethylbutane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37	-128.54
11	Heptane	98.427	146.540	34.5504	36,55	267.55	27.01	20.26	-90.61
12	2-methylhexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29	-118.28
13	3-methylhexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-118.60
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247,70	28.4	18.02	-123.81
16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
17	2,4-dimethylpentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15	-119.24
18	3,3-dimethylpentane	86.064	144.430	34.3323	33.02	263.00	30	19.59	-134.46
19	Octane	125.665	162.592	39.1922	41.48	296.20	24,64	21.76	-56.79
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
21	3-methylheptane	118.925	161.832	39.1001	39.83	282.00	25.6	21.17	-120.50
22	4-methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95
23	3- ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51	
24	2,2-dimethylhexane	10.84	164.28	37.29	37.29	279.00	25.6	19.60	-121.18
25	2,3-dimethylhexane	115.607	160.39	38.79	38.79	293.00	26.6	20.99	
26	2,4-dimethylhexane	109.42	163.09	37.76	37.76	282.00	25.8	20.05	-137.50
27	2,5-dimethylhexane	109.10	164.69	37.86	37.86	279.00	25	19.73	-91.20
28	3,3- dimethylhexane	111.96	160.87	37.93	37.93	290.84	27.2	20.63	-126.10
29	3,4-dimethylhexane	117.72	158.81	39.02	39.02	298.00	27.4	21.64	
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52	-114.96
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99	-90.87
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67	-112.27
33	2,2,4-trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	-107.38
34	2,3,3-trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56	-100.70

35	2,3,4-trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14	-109.21
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92	-53.52
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88	-80.40
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34	-107.64
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34	-113.20
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81	-114.90
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81	
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80	-113.00
43	2,3-dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34	-116.00
44	2,4-dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30	
45	2,5-dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30	
46	2,6-dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83	-102.90
47	3,3-dimethylheptane	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
48	3,4-dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
49	3,5-dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
50	4,4-dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.56	23.22	
54	2,2,4-trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5-trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3-trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4-trimethylhexane	139.00	173.498	43.4917	42.93	324.20	25.46	22.80	
58	2,3,5-trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4-trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0

65	2,2,3,4-tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4-tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-66.54
67	2,3,3,4-tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12

3. Regression Models

The following statistical models have been used for the study:

- Linear Model: $P = aX + b$,
- Quadratic Model: $P = aX^2 + bX + c$,
- Logarithmic Model: $P = a + b\ ln(x)$,

where P is a physical property, X is a domination parameter, a, b and c are constants. Now, we have obtained the following different regression models for each parameter, which are listed below.

4. F-Sombor Index(FSLI)

1. Linear Model

$$bp = 2.055 + [FSLI]29.5 \quad (1)$$

$$mv = -1.104 + [FSLI]33.5 \quad (2)$$

$$mr = 0.187 + [FSLI]26.3 \quad (3)$$

$$v = 0.189 + [FSLI]25.5 \quad (4)$$

$$ct = 3.469 + [FSLI]177.9 \quad (5)$$

$$cp = 39.875 - [FSLI]6.4 \quad (6)$$

$$st = 0.098 + [FSLI]18.7 \quad (7)$$

$$mp = -123.759 + [FSLI]0.457 \quad (8)$$

2. Quadratic Model

$$bp = 5.9[FSLI]^2 - 0.02[FSLI] - 50.6 \quad (9)$$

$$mv = 2.4[FSLI]^2 - 0.007\ [FSLI] + 91.1 \quad (10)$$

$$mr = 0.3[FSLI]^2 - 0.003[FSLI] + 19.2 \quad (11)$$

$$hv = 0.4[FSLI]^2 - 0.004[FSLI] + 20.1 \quad (12)$$

$$ct = 4.9[FSLI]^2 - 0.09[FSLI] + 105.7 \quad (13)$$

$$cp = -0.4[FSLI]^2 + 0.003[FSLI] + 38.2 \quad (14)$$

$$st = 0.3[FSLI]^2 - 0.002[FSLI] + 15.1 \quad (15)$$

$$mp = 0.7[FSLI]^2 - 0.007[FSLI] + 149.2 \quad (16)$$

3. Logarithmic Model

$$bp = 64.9 - ln[FSLI]167.4 \quad (17)$$

$$mv = 66.8 + ln[FSLI]74.5 \quad (18)$$

$$mr = 8.9 + ln[FSLI]27.1 \quad (19)$$

$$hv = 11.4 + ln[FSLI]23.2 \quad (20)$$

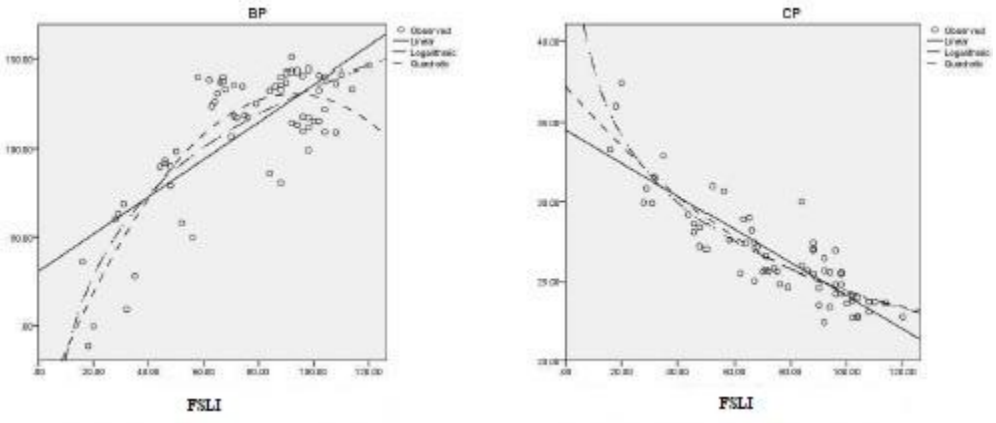
$$ct = 12.07 - ln[FSLI]9.1 \quad (21)$$

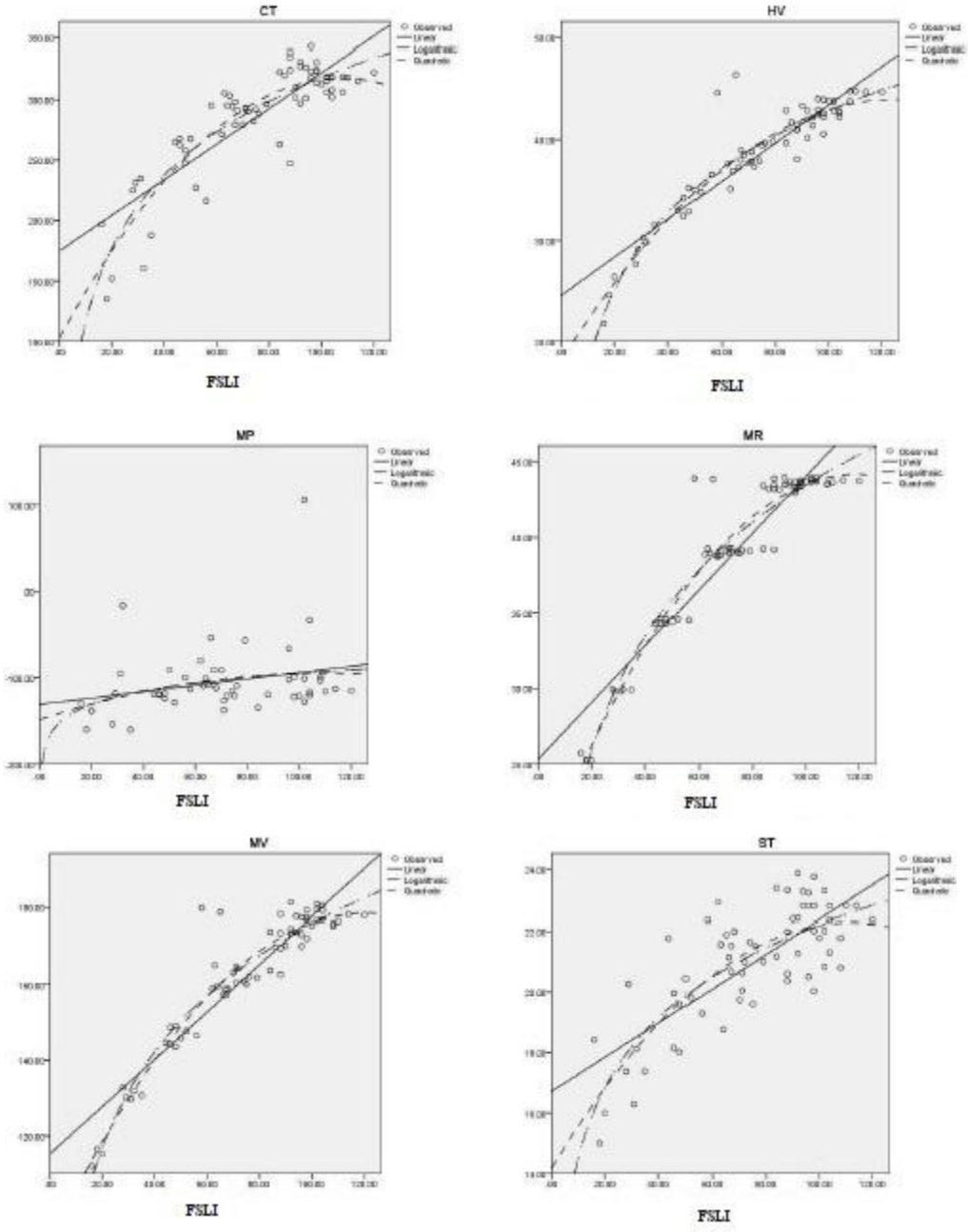
$$cp = -8.06 - ln[FSLI]51.3 \quad (22)$$

$$\text{st} = 10.06 + ln[FSLI]8.3 \quad (23)$$

$$\text{mp} = 21.1 - ln[FSLI]199.7 \quad (24)$$

In the following figures, the correlation of F-Sombor Index with above mentioned physical properties of alkanes are shown:




CT
HV
MP
MR
MV
ST
FSLI

5. Sum Connectivity Gourava Index (SCGI)

1. Linear Model

$$bp = -46.450 + [SCGI]0.379 \quad (25)$$

$$mv = 78.533 + [SCGI]0.283 \quad (26)$$

$$mr = 10.916 + [SCGI]1.412 \quad (27)$$

$$hv = 14.435 + [SCGI]10.457 \quad (28)$$

$$ct = 99.561 + [SCGI]10.457 \quad (29)$$

$$cp = 28.113 - [SCGI]0.235 \quad (30)$$

$$st = 25.256 + [SCGI]0.529 \quad (31)$$

$$mp = -174.768 + [SCGI]2.436 \quad (32)$$

2. Quadratic Model

$$bp = 10.567[SCGI]^2 - 0.884[SCGI] - 132.568 \quad (33)$$

$$mv = 7.876[SCGI]^2 - 0.143\,[SCGI] + 60.263 \quad (34)$$

$$mr = 3.132[SCGI]^2 - 0.052[SCGI] + 31.184 \quad (35)$$

$$hv = 3.448[SCGI]^2 - 0.075[SCGI] + 11.971 \quad (36)$$

$$ct = 36.365[SCGI]^2 - 0.625[SCGI] + 18.542 \quad (37)$$

$$cp = -7.363[SCGI]^2 + 0.047[SCGI] + 56.6\,92 \quad (38)$$

$$st = 0.967[SCGI]^2 - 0.010[SCGI] + 13.482 \quad (39)$$

$$mp = 2.732[SCGI]^2 - 0.047[SCGI] - 149.002 \quad (40)$$

3. Logarithmic Model

$$bp = -194.741 - ln[SCGI]100.176 \quad (41)$$

$$mv = 9.017 + ln[SCGI]64.949 \quad (42)$$

$$mr = -3.628 + ln[SCGI]19.187 \quad (43)$$

$$hv = -7.376 + ln[SCGI]12.107 \quad (44)$$

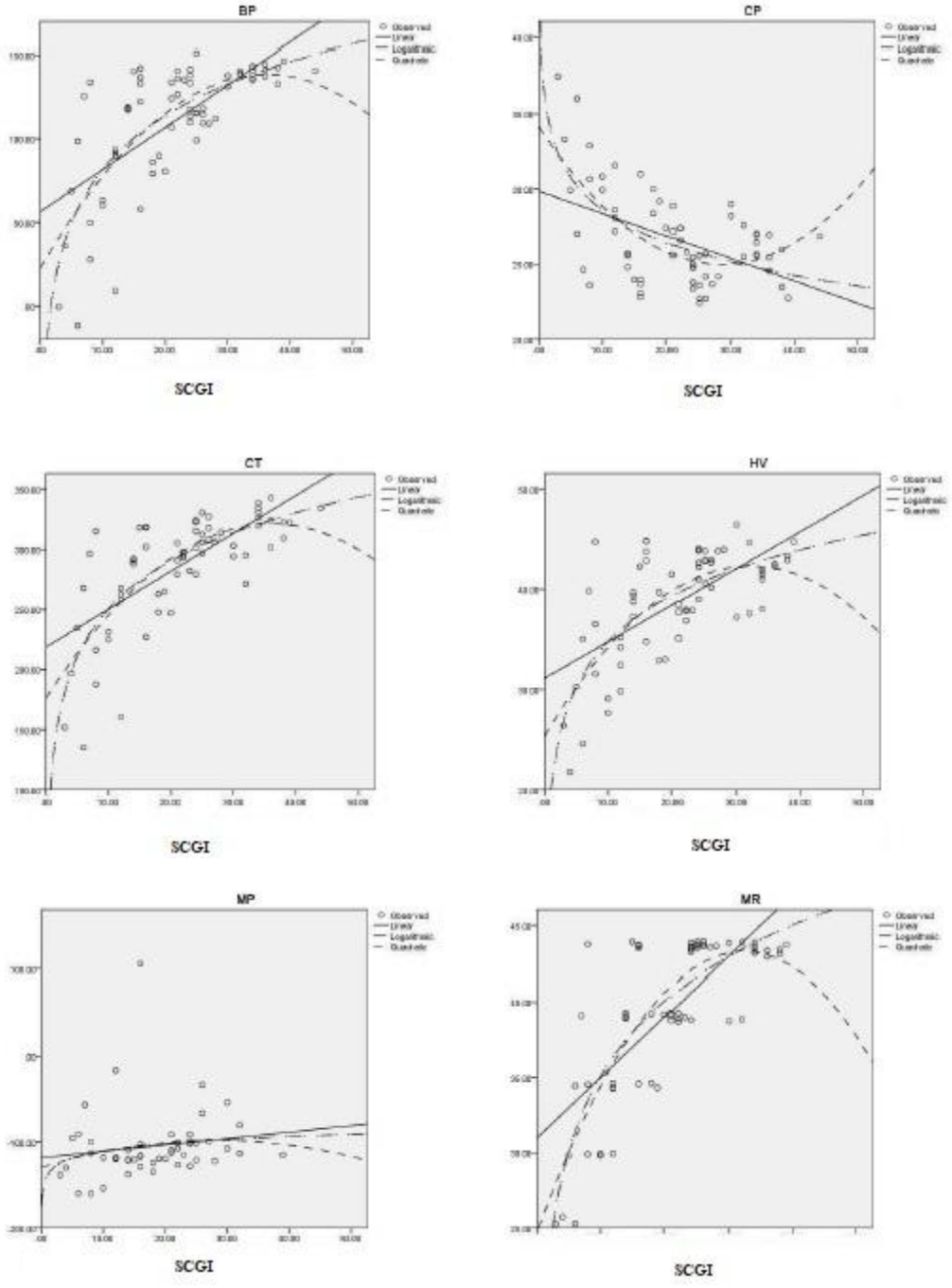
$$ct = -117.478 + ln[SCGI]165.712 \quad (45)$$

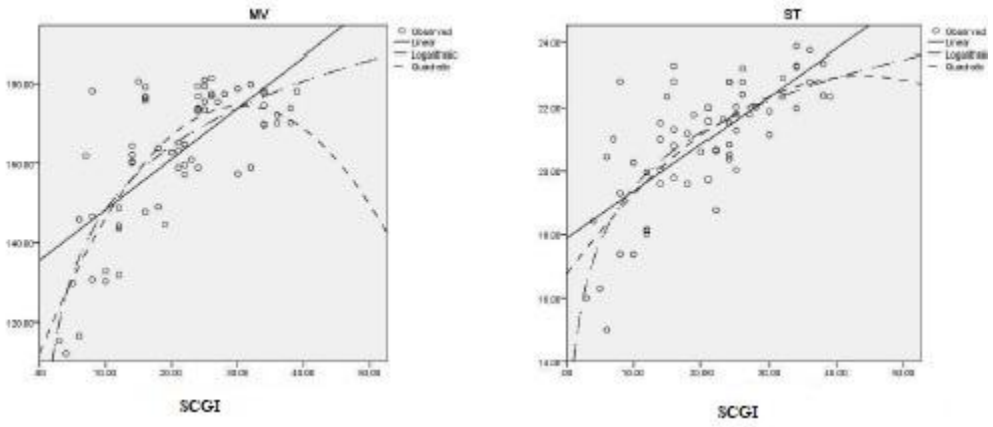
$$cp = 55.929 - ln[SCGI]10.959 \quad (46)$$

$$st = 6.786 + ln[SCGI]7.458 \quad (47)$$

$$mp = -210.472 + ln[SCGI]35.081 \qquad (48)$$

In the following figures, the correlation of sum connectivity Gourava index with abovementioned physical properties of alkanes are shown:





6. Product Connectivity Gourava Index (PCGI)

1. Linear Model

$$bp = 5.194 + [PCGI]4.554 \quad (49)$$

$$mv = 107.456 + [PCGI]0.870 \quad (50)$$

$$mr = 23.218 + [PCGI]1.456 \quad (51)$$

$$hv = 23.909 + [PCGI]0.886 \quad (52)$$

$$ct = 123.038 + [PCGI]4.317 \quad (53)$$

$$cp = 57.082 - [PCGI]0.248 \quad (54)$$

$$st = 13.125 + [PCGI]0.578 \quad (55)$$

$$mp = -145.961 + [PCGI]1.265 \quad (56)$$

2. Quadratic Model

$$bp = 11.9[PCGI]^2 - 0.12[PCGI] - 47.612 \quad (57)$$

$$mv = 4.654[PCGI]^2 - 0.042[PCGI] + 88.216 \quad (58)$$

$$mr = 1.132[PCGI]^2 - 0.15[PCGI] + 18.132 \quad (59)$$

$$hv = 1.316[PCGI]^2 - 0.015[PCGI] + 14.259 \quad (60)$$

$$ct = 10.192[PCGI]^2 - 0.0101[PCGI] + 78.430 \quad (61)$$

$$cp = -0.980[PCGI]^2 + 0.014[PCGI] + 23.965 \quad (62)$$

$$st = 0.340[PCGI]^2 - 0.008[PCGI] + 23.456 \quad (63)$$

$$mp = 2.613[PCGI]^2 - 0.25[PCGI] - 134.608 \quad (64)$$

3. Logarithmic Model

$$bp = -147.275 - ln[PCGI]78.903 \quad (65)$$

$$mv = 45.434 + ln[PCGI]40.210 \quad (66)$$

$$mr = 0.876 + ln[PCGI]10.236 \quad (67)$$

$$hv = 21.608 + ln[PCGI]0.655 \quad (68)$$

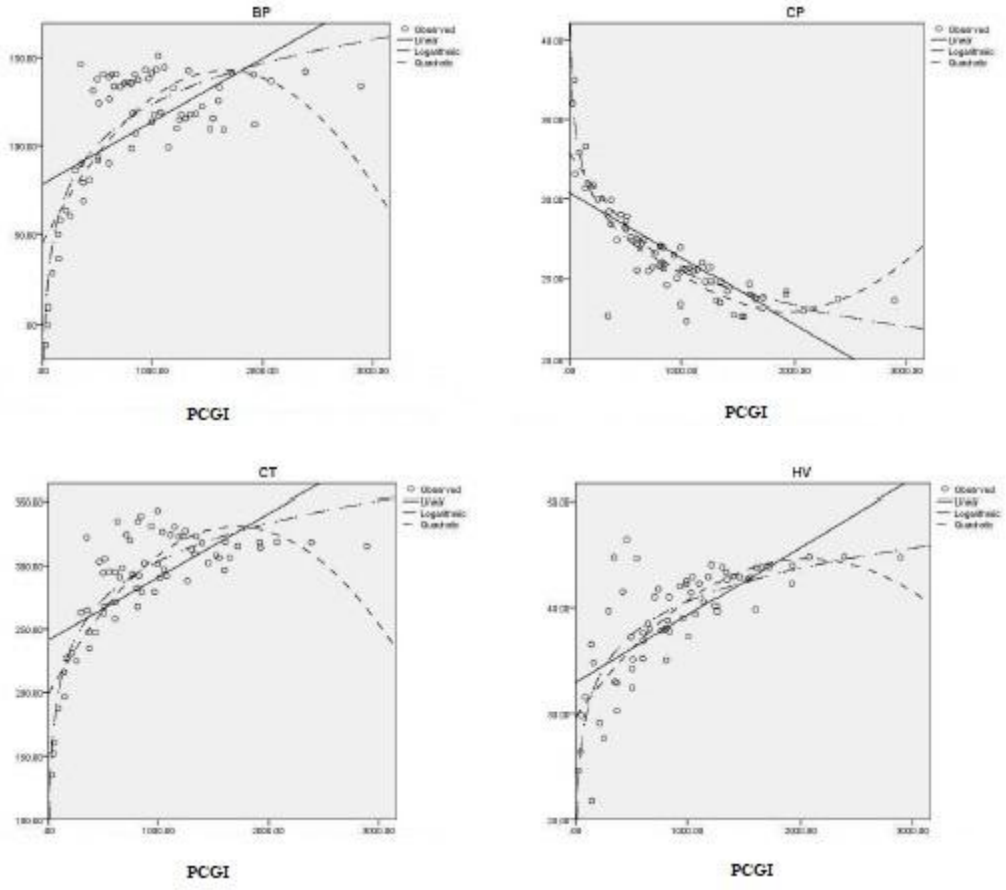
$$ct = -50.591 + ln[PCGI]100.567 \quad (69)$$

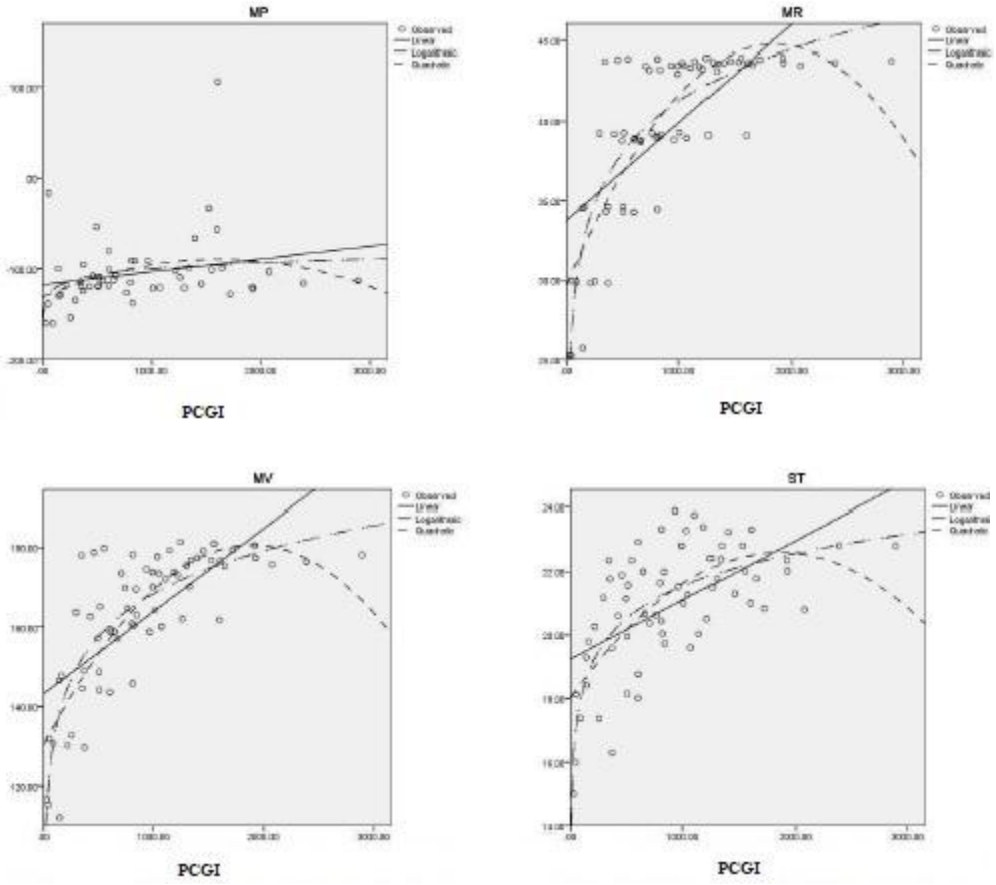
$$cp = 44.853 - ln[PCGI]4.139 \quad (70)$$

$$st = 5.452 + ln[PCGI]3.511 \quad (71)$$

$$mp = -186.817 + ln[PCGI]18.221 \quad (72)$$

In the following figures, the correlation of product connectivity Gourava index with above mentioned physical properties of alkanes are shown:





7. Multiplicative Atom Bond Sum Connectivity Index(MASCI)

1. Linear Model

$$bp = -56.617 + [MASCI]36.785 \quad (73)$$

$$mv = 75.043 + [MASCI]13.988 \quad (74)$$

$$mr = 14.070 + [MASCI]5.401 \quad (75)$$

$$hv = 16.809 + [MASCI]5.912 \quad (76)$$

$$ct = 74.987 + [MASCI]35.537 \quad (77)$$

$$cp = 37.578 - [MASCI]3.013 \quad (78)$$

$$st = 15.540 + [MASCI]2.435 \quad (79)$$

$$mp = -158.005 + [MASCI]10.104 \quad (80)$$

2. Quadratic Model

$$bp = 78.544[MASCI]^2 - 4.622[MASCI] - 168.756 \quad (81)$$

$$mv = 51.766[MASCI]^2 - 4.004[MASCI] + 14.767 \quad (82)$$

$$mr = 10.465[MASCI]^2 - 0.178[MASCI] - 1.474 \quad (83)$$

$$hv = 12.506[MASCI]^2 - 1.050[MASCI] + 4.654 \quad (84)$$

$$ct = 124.251[MASCI]^2 - 8.838[MASCI\ ] - 110.078 \quad (85)$$

$$cp = -10.902[MASCI]^2 + 0.879[MASCI] + 56.177 \quad (86)$$

$$st = 3.676[MASCI]^2 - 0.253[MASCI] + 5.254 \quad (87)$$

$$mp = 12.231[MASCI]^2 - 0.881[MASCI] - 156.446 \quad (88)$$

3. Logarithmic Model

$$bp = -165.05 - ln[MASCI]132.211 \quad (89)$$

$$mv = 45.460 + ln[MASCI]56.637 \quad (90)$$

$$mr = 0.876 + ln[MASCI]12.235 \quad (91)$$

$$hv = 7.204 + ln[MASCI]16.929 \quad (92)$$

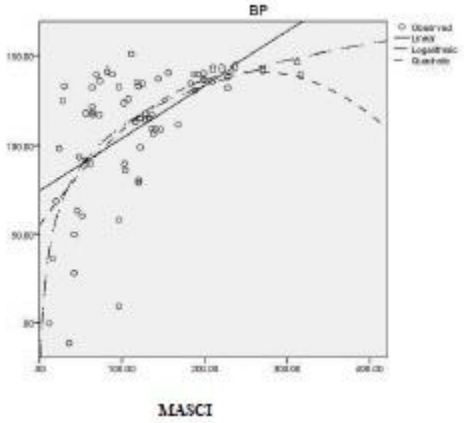
$$ct = -55.591 + ln[MASCI]110.013 \quad (93)$$

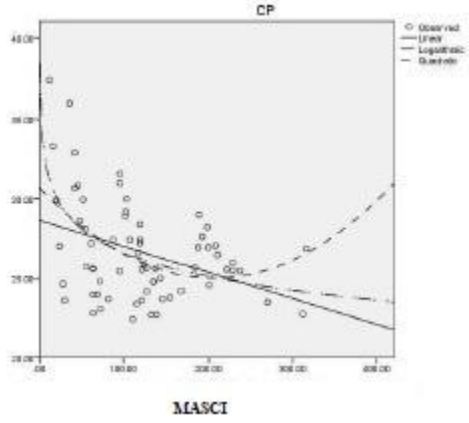
$$cp = 42.629 - ln[MASCI]10.323 \quad (94)$$

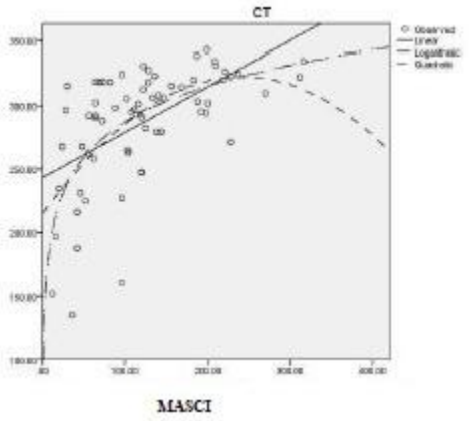
$$st = 10.567 + ln[MASCI]4.725 \quad (95)$$

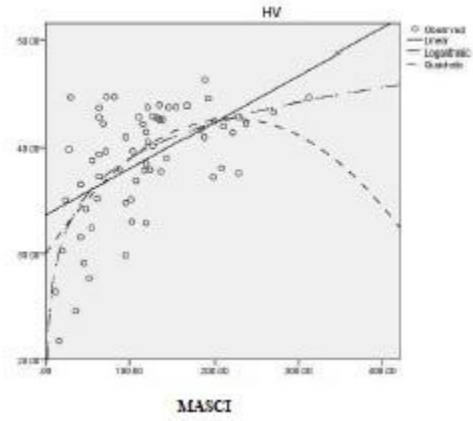
$$mp = -162.580 + ln[MASCI]47.054 \quad (96)$$

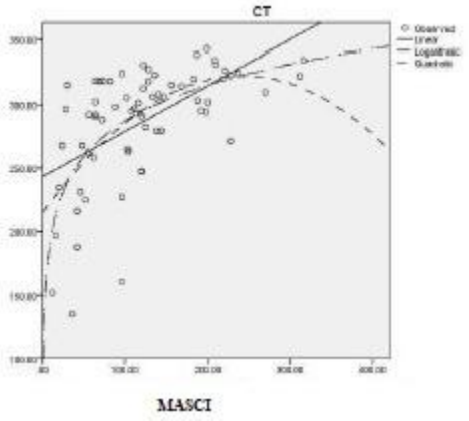
In the following figures, the correlation of multiplicative atom bond sum connectivity index with above mentioned physical properties of alkanes are shown:

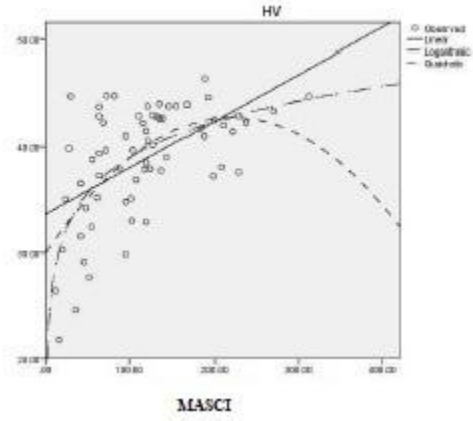


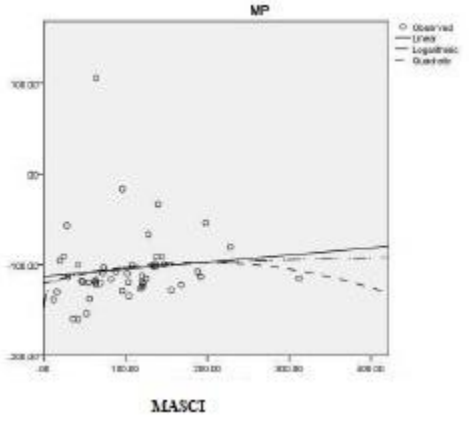


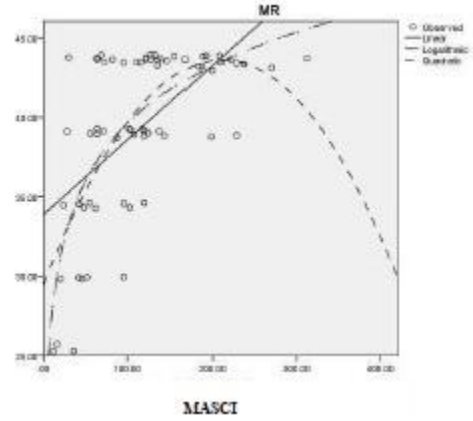

CT
MASCI

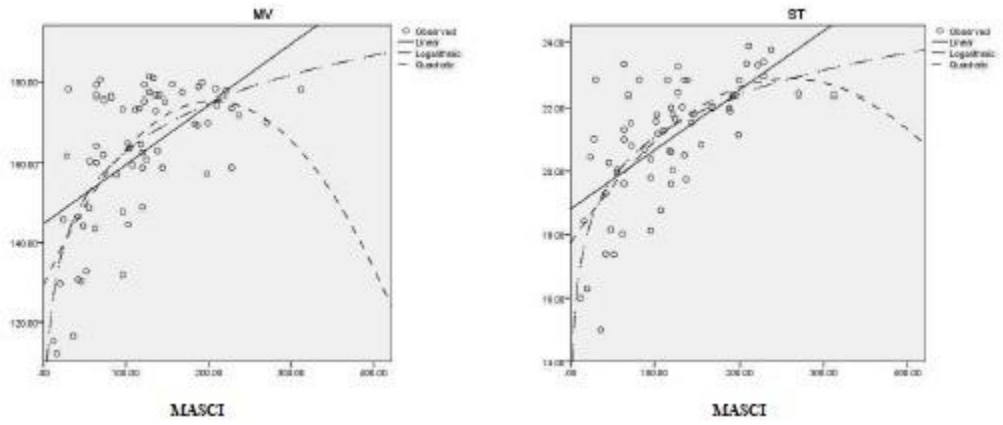

HV
MASCI


CT
MASCI


HV
MASCI


MP
MASCI


MR
MASCI



8. Sum Augmented Index (SAI)

1. Linear Model

$$bp = 11.536 + [SAI]1.351 \quad (97)$$

$$mv = 110.932 + [SAI]1.086 \quad (98)$$

$$mr = 30.569 + [SAI]0.213 \quad (99)$$

$$hv = 21.315 + [SAI]0.328 \quad (100)$$

$$ct = 151.329 + [SAI]3.201 \quad (101)$$

$$cp = 32.467 - [SAI]0.280 \quad (102)$$

$$st = 14.205 + [SAI]0.199 \quad (103)$$

$$mp = -131.576 + [SAI]0.276 \quad (104)$$

2. Quadratic Model

$$bp = 5.23[SAI]^2 - 0.036[SAI] - 78.089 \quad (105)$$

$$mv = 1.446[SAI]^2 - 0.008[SAI] + 101.796 \quad (106)$$

$$mr = 0.625[SAI]^2 - 0.001[SAI] + 19.575 \quad (107)$$

$$hv = 0.615[SAI]^2 - 0.001[SAI] + 22.595 \quad (108)$$

$$ct = 6.22[SAI]^2 - 0.035[SAI] + 55.987 \quad (109)$$

$$cp = -0.979[SAI]^2 + 0.002[SAI] + 28.205 \quad (110)$$

$$st = 0.416[SAI]^2 - 0.001[SAI] + 13.182 \quad (111)$$

$$mp = -2.241[SAI]^2 - 0.053[SAI] - 74.870 \quad (112)$$

3. Logarithmic Model

$$bp = -177.566 + ln[SAI]80.881 \quad (113)$$

$$mv = 27.459 + ln[SAI]34.302 \quad (114)$$

$$mr = -0.988 + ln[SAI]10.396 \quad (115)$$

$$hv = 0.359 + ln[SAI]10.402 \quad (116)$$

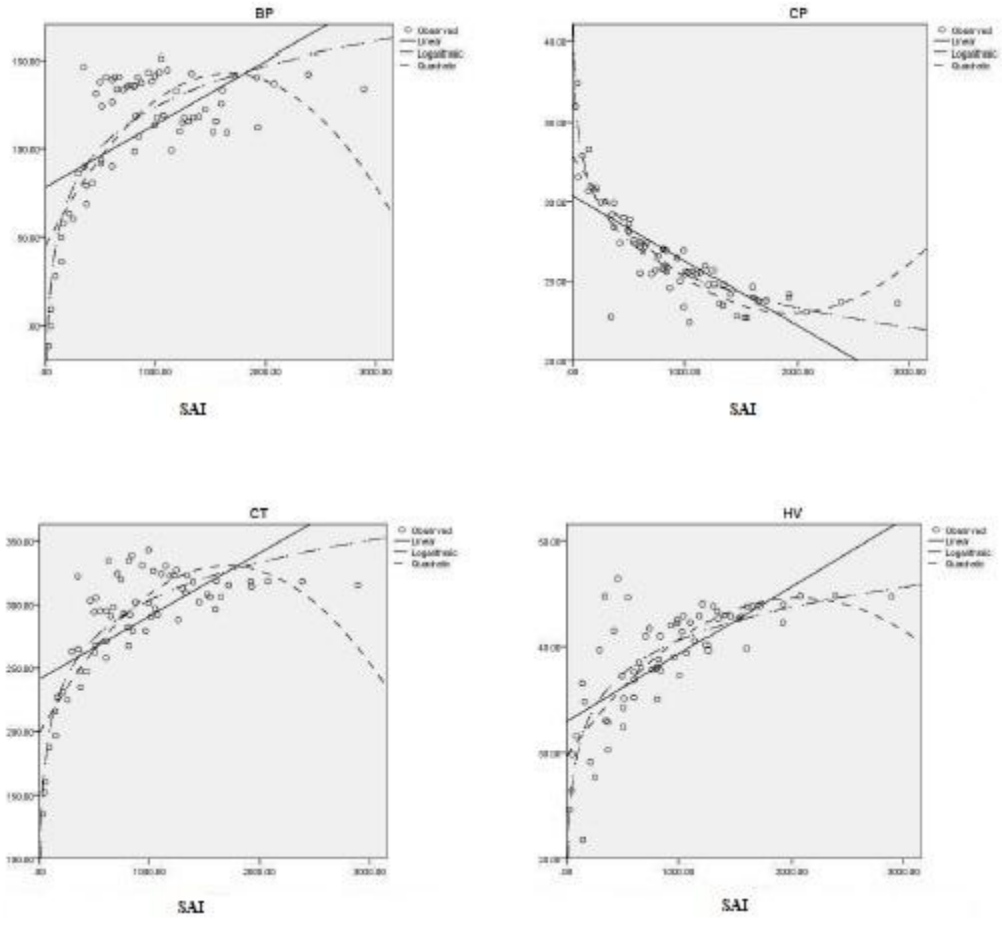
$$ct = -131.812 + ln[SAI]106.234 \quad (117)$$

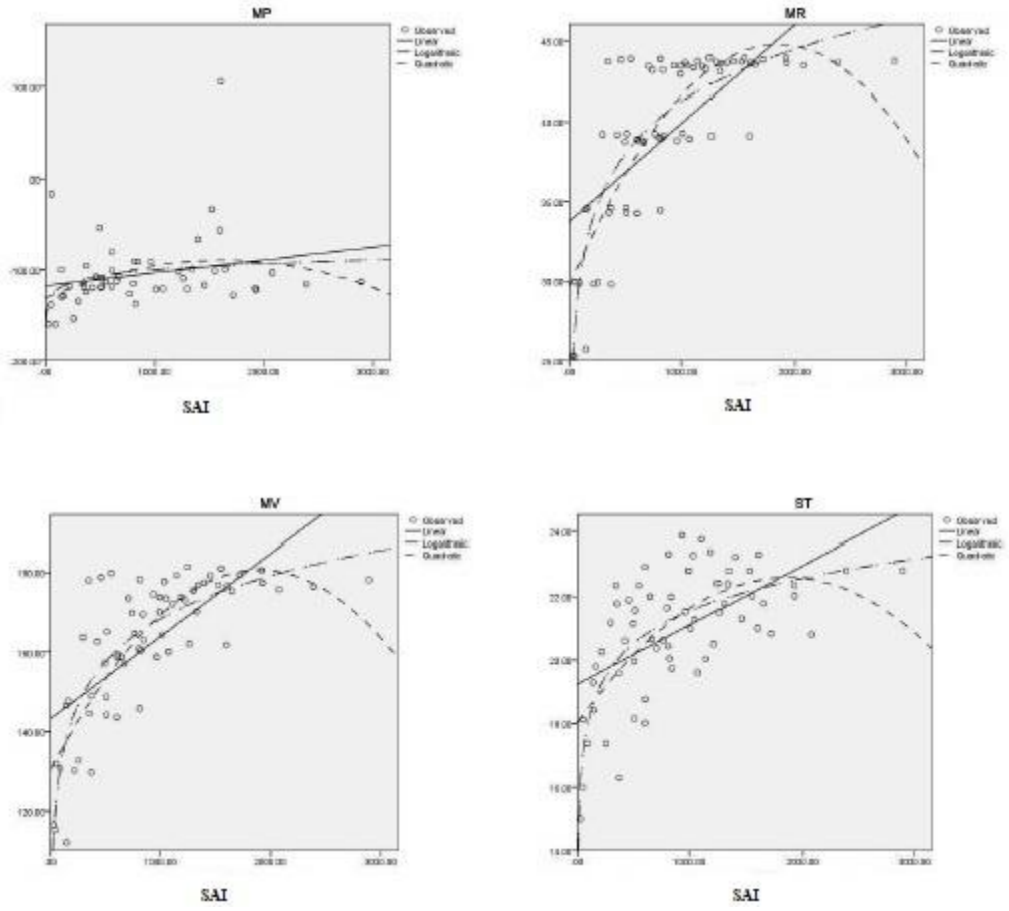
$$cp = 49.847 - ln[SAI]49.847 \quad (118)$$

$$st = 9.067 + ln[SAI]3.241 \quad (119)$$

$$mp = -148.213 + ln[SAI]16.200 \quad (120)$$

In the following figures, the correlation of sum augmented index with above mentioned physical properties of alkanes are shown:





9. Revan Sombor Index (RSI)

1. Linear Model

$$bp = -43.940 + [RSI]24.445 \quad (121)$$

$$mv = 78.145 + [RSI]10.557 \quad (122)$$

$$mr = 17.101 + [RSI]4.777 \quad (123)$$

$$hv = 14.673 + [RSI]2.454 \quad (124)$$

$$ct = 70.271 + [RSI]31.564 \quad (125)$$

$$cp = 39.667 - [RSI]2.102 \quad (126)$$

$$st = 12.563 + [RSI]2.01 \quad (127)$$

$$mp = -149.282 + [RSI]6.457 \quad (128)$$

2. Quadratic Model

$$bp = 82.320[RSI]^2 - 3.141[RSI] - 200.458 \quad (129)$$

$$mv = 10.019[RSI]^2 + 0.123[RSI] + 78.479 \quad (130)$$

$$mr = 3.624[RSI]^2 - 0.013[RSI] + 13.501 \quad (131)$$

$$hv = 2.234[RSI]^2 + 0.061[RSI] + 17.346 \quad (132)$$

$$ct = 61.467[RSI]^2 - 2.567[RSI] - 10.167 \quad (133)$$

$$cp = -3.002[RSI]^2 + 0.078[RSI] + 43.276 \quad (134)$$

$$st = 2.754[RSI]^2 - 0.134[RSI] + 10.012 \quad (135)$$

$$mp = -14.348[RSI]^2 + 1.998[RSI] - 87.176 \quad (136)$$

3. Logarithmic Model

$$bp = -139.117 + ln[RSI]136.276 \quad (137)$$

$$mv = 42.457 + ln[RSI]64.795 \quad (138)$$

$$mr = 3.356 + ln[RSI]18.456 \quad (139)$$

$$hv = 4.367 + ln[RSI]17.187 \quad (140)$$

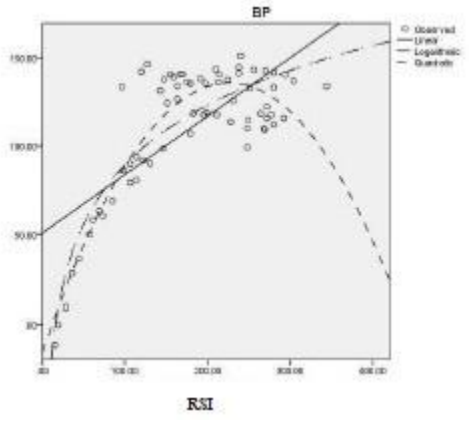
$$ct = -39.742 + ln[RSI]177.812 \quad (141)$$

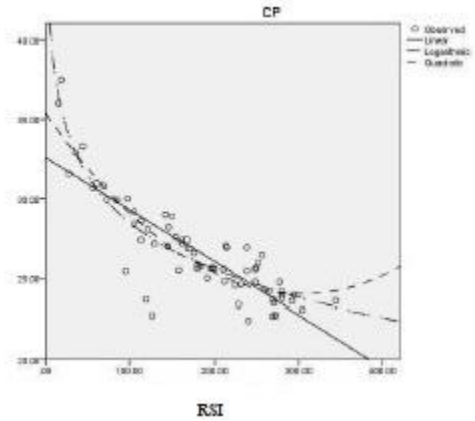
$$cp = 46.467 - ln[RSI]10.419 \quad (142)$$

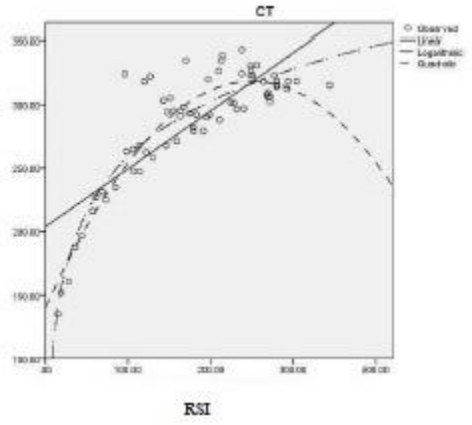
$$st = 8.999 + ln[RSI]7.672 \quad (143)$$

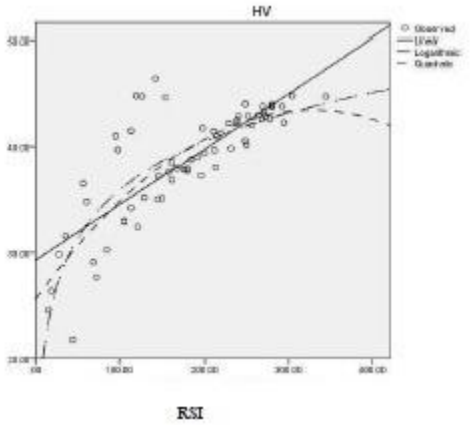
$$mp = -189.470 + ln[RSI]37.627 \quad (144)$$

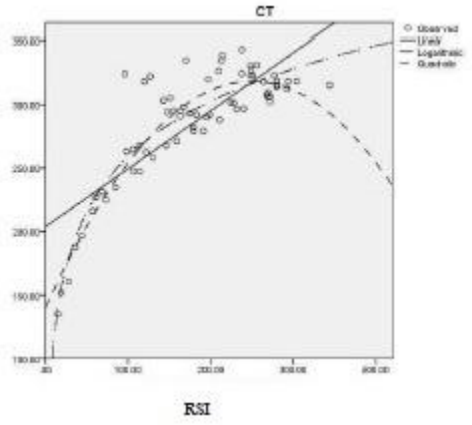
In the following figures, the correlation of Revan Sombor index with above mentioned physical properties of alkanes are shown:

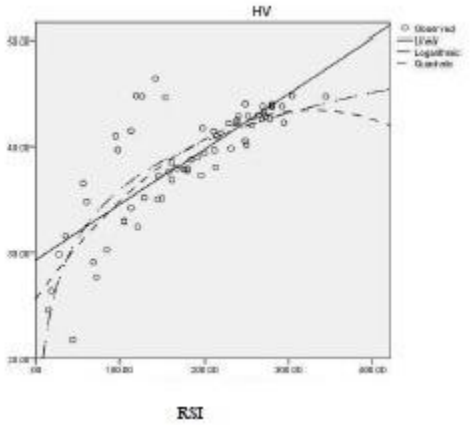


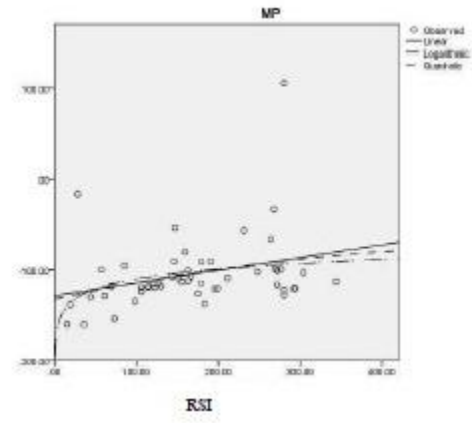


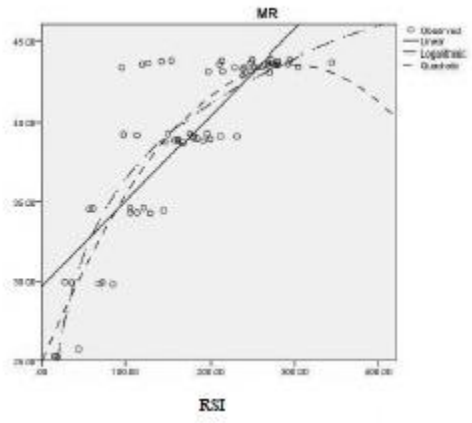

CT
RSI

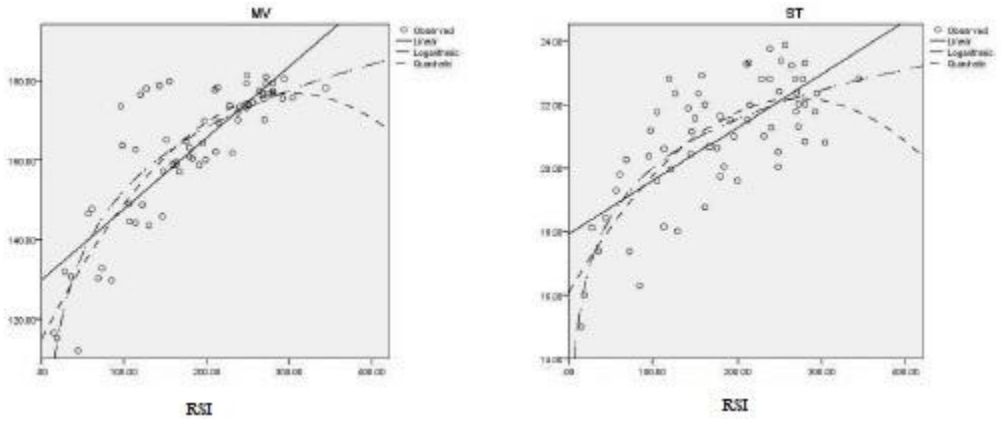

HV
RSI


CT
RSI


HV
RSI


MP
RSI


MR
RSI



10. Discussion and Concluding Remark

By inspection of the data given in tables 1 and 2, and equations (7)-(150) it is possible to draw a number of conclusions for the given domination parameters.

- The F-Sombor index(FSLI) is the first has correlation coefficient value ranging from 0.071 to 0.88 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar volume of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.084 to 0.9 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refraction of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.074 to 0.921 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refraction of alkanes respectively.
- The sum connectivity Gourava index(SCGI) plays an important role in QSPR studies of alkanes. The correlation coefficient value ranges from 0.023 to 0.523 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.091 to 0.76 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.054 to 0.78 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively.

- The product connectivity Gourava index (PCGI) shows better predicting power than the connected domination number. The correlation coefficient value ranges from 0.055 to 0.698 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.077 to 0.891 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.088 to 0.895 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively.
- The multiplicative atom bond sum connectivity Index (MASCI) found to be useful parameter in QSPR-studies. The correlation coefficient value ranges from 0.092 to 0.867 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical pressure of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.098 to 0.897 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.09 to 0.923 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.
- The sum augmented index (SAI) found to be less useful domination parameter compare to the total domination number. The correlation coefficient value ranges from 0.035 to 0.478 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for surface tension of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.033 to 0.779 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.021 to 0.793 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.
- The Revan Sombor index (RSI) has a good predictive power for the set of alkanes. The correlation coefficient value ranges from 0.086 to 0.967 for linear model with minimum

correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.091 to 0.578 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.062 to 0.578 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for molar refractions of alkanes respectively.

11. Conclusion.

From practical point of view, topological indices for which the absolute value of correlation coefficient is less than 0.8 can be characterized as useless. Overall, the molecular descriptors considered for this study are useful candidates to predict the critical temperature of alkanes.

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