Malaya Journal of Matematik, Vol. 8, No. 1, 314-330, 2020

https://doi.org/10.26637/MJM0802/0003

QSPR analysis of Alkanes with certain degree based topological indices

K.N. Anil Kumar[1], N.S. Basavarajappa [2*] and M.C. Shanmukha [3]

Abstract

The topological indices are the important tools in QSPR studies. Recently Hosamani et. al., [11] studied the QSPR analysis of some degree based topological indices by selecting the linear model: $P = a + (TI)b$, where P is the physical property and TI is the topological index. In this paper, we carry forward their work by studying the quadratic and logarithmic models for the set 67 alkanes.

Keywords

Topological indices, QSPR-analysis, octane isomers.

AMS Subject Classification

05C90, 05C35, 05C12.

[1,2] *Department of Mathematics, Bapuji Institute of Engineering and Technology, Davanagere- 577004, Karnataka, India and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka, India.*

[3] *Department of Mathematics, Jain Institute of Technology, Davanagere- 577003, Karnataka, India and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka, India.*

***Corresponding author**: [2]dr.nsbasavaraj@gmail.com; [3]mcshanmukha@gmail.com; [1]kn.anil5340@gmail.com

Article History: Received **27** September **2019**; Accepted **15** March **2020**

Contents

1. Introduction

The topological indices are a 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. In this paper, we have considered the following topological indices for the QSPR study.

Randić Index [13]

$$R(G) = \sum_{u\sim v} \frac{1}{\sqrt{d_G(u)d_G(v)}} \tag{1.1}$$

Reciprocal Randić Index [13]

$$RR(G) = \sum_{u\sim v} \sqrt{d_G(u)d_G(v)}. \tag{1.2}$$

Second Zagreb Index [4]

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v) \tag{1.3}$$

Atom-Bond Connectivity Index [1]

$$ABC(G) = \sum_{u\sim v} \sqrt{\frac{d_u(G)+d_v(G)-2}{d_u(G)d_v(G)}} \tag{1.4}$$

Augumented Zagreb Index [3]

$$AZI(G) = \sum_{uv\in E(G)}\left(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}\right)^3. \quad (1.5)$$

Geometric-Airthmetic Index [14]

$$GA(G) = \sum_{u\sim v}\frac{2\sqrt{d_u(G)d_v(G)}}{d_u(G)+d_v(G)} \quad (1.6)$$

Harmonic Index [2]

$$H(G) = \sum_{u\sim v}\frac{2}{d_u(G)+d_v(G)} \quad (1.7)$$

Sum Connectivity Index [15]

$$SCI(G) = \sum_{u\sim v}\frac{1}{d_u(G)+d_G(v)} \quad (1.8)$$

For recent work on degree-based topological indices, we refer the interested reader to the articles [5–10, 12].

2. The Use of Selected Degree Based Topological Indices in QSPR Studies

We have used here 08 degree based topological indices, viz., $M_2(G), R(G), ABC(G), AZI(G), GA(G), H(G), SCI(G)\, RR(G)$ for modeling 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 these property were taken from [11]. The values are compiled in Table 1 and Table [2] in [11].

3. Regression Models

The following statistical models have been used for the study:

- Linear Model:

$$P = a(TI)+b \quad (3.1)$$

- Quadratic Model :

$$P = a(TI)^2+b(TI)+c \quad (3.2)$$

- Logarithmic Model:

$$P = a+b\ln(TI) \quad (3.3)$$

where P is a physical property, TI is a topological index and a, b and c are constants.

Now we have obtained the following different regression models for each degree based topological index, which are listed below.

4. Randić index $R(G)$

1. Linear Model

$$\begin{aligned} bp &= -76.519+[R(G)]51.433\\ mv &= 71.458+[R(G)]24.968\\ mr &= 11.965+[R(G)]7.546\\ hv &= 12.352+[R(G)]7.270\\ ct &= 39.946+[R(G)]68.560\\ cp &= 42.875-[R(G)]4.459\\ st &= 12.463+[R(G)]2.337\\ mp &= -160.901+[R(G)]15.931 \end{aligned}$$

2. Quadratic Model

$$\begin{aligned} bp &= 199.335[R(G)]^2-22.750[R(G)]-304.298\\ mv &= 22.884[R(G)]^2+0.320[R(G)]+74.660\\ mr &= 7.546[R(G)]^2-7.526[R(G)]+11.964\\ hv &= 5.351[R(G)]^2+0.295[R(G)]+15.307\\ ct &= 156.322[R(G)]^2-13.499[R(G)]-98.213\\ cp &= -7.446[R(G)]^2+0.459[R(G)]+47.975\\ st &= 4.948[R(G)]^2-0.401[R(G)]+8.444\\ mp &= -39.589[R(G)]^2+8.559[R(G)]-76.219 \end{aligned}$$

3. Logarithmic Model

$$\begin{aligned} bp &= -98.213+\ln[R(G)]164.078\\ mv &= 64.861+\ln[R(G)]76.576\\ mr &= 9.942+\ln[R(G)]23.165\\ hv &= 10.487+\ln[R(G)]22.253\\ ct &= 11.673+\ln[R(G)]7.305\\ cp &= 44.262-\ln[R(G)]13.873\\ st &= 11.673+\ln[R(G)]7.305\\ mp &= -161.902+\ln[R(G)]46.179 \end{aligned}$$

5. Reciprocal Randić Index $RR(G)$

1. Linear Model

$$\begin{aligned} bp &= -36.550+[RR(G)]10.479\\ mv &= 88.599+[RR(G)]5.283\\ mr &= 10.916+[RR(G)]1.613\\ hv &= 17.878+[RR(G)]1.5\\ ct &= 94.651+[RR(G)]13.654\\ cp &= 38.098-[RR(G)]0.815\\ st &= 13.613+[RR(G)]0.529\\ mp &= -154.694+[RR(G)]3.816 \end{aligned}$$

2. Quadratic Model

$$\begin{aligned}
bp &= 29.569[RR(G)]^2 - 0.777[RR(G)] - 143.624\\
mv &= 8.562[RR(G)]^2 - 0.135[RR(G)] + 70.362\\
mr &= 2.231[RR(G)]^2 - 0.025[RR(G)] + 13.481\\
hv &= 2.884[RR(G)]^2 - 0.057[RR(G)] + 10.179\\
ct &= 26.563[RR(G)]^2 - 0.526[RR(G)] + 22.245\\
cp &= -2.633[RR(G)]^2 + 0.074[RR(G)] + 48.296\\
st &= 0.769[RR(G)]^2 - 0.010[RR(G)] + 12.284\\
mp &= 2.732[RR(G)]^2 - 0.047[RR(G)] - 149.022
\end{aligned}$$

3. Logarithmic Model

$$\begin{aligned}
bp &= -204.147 + \ln[RR(G)]120.671\\
mv &= 10.071 + \ln[RR(G)]58.499\\
mr &= -6.826 + \ln[RR(G)]17.771\\
hv &= -4.673 + \ln[RR(G)]16.701\\
ct &= -115.874 + \ln[RR(G)]154.217\\
cp &= 51.429 - \ln[RR(G)]9.499\\
st &= 5.777 + \ln[RR(G)]5.844\\
mp &= -206.274 + \ln[RR(G)]40.018
\end{aligned}$$

6. Second Zagreb index $M_2(G)$

1. Linear Model

$$\begin{aligned}
bp &= 3.194 + [M_2(G)]3.582\\
mv &= 108.696 + [M_2(G)]1.806\\
mr &= 22.911 + [M_2(G)]0.556\\
hv &= 23.808 + [M_2(G)]0.505\\
ct &= 145.038 + [M_2(G)]4.713\\
cp &= 34.082 - [M_2(G)]0.248\\
st &= 15.125 + [M_2(G)]0.198\\
mp &= -144.169 + [M_2(G)]1.462
\end{aligned}$$

2. Quadratic Model

$$\begin{aligned}
bp &= 9.5[M_2(G)]^2 - 0.11[M_2(G)] - 67.612\\
mv &= 4.654[M_2(G)]^2 - 0.042[M_2(G)] + 82.216\\
mr &= 1.132[M_2(G)]^2 - 0.11[M_2(G)] + 16.132\\
hv &= 1.316[M_2(G)]^2 - 0.015[M_2(G)] + 14.259\\
ct &= 10.197[M_2(G)]^2 - 0.0101[M_2(G)] + 79.430\\
cp &= -0.990[M_2(G)]^2 + 0.014[M_2(G)] + 42.965\\
st &= 0.340[M_2(G)]^2 - 0.003[M_2(G)] + 13.466\\
mp &= 2.612[M_2(G)]^2 - 0.25[M_2(G)] - 155.608
\end{aligned}$$

3. Logarithmic Model

$$\begin{aligned}
bp &= -157.572 + \ln[M_2(G)]80.309\\
mv &= 35.344 + \ln[M_2(G)]38.120\\
mr &= 0.678 + \ln[M_2(G)]11.632\\
hv &= 23.808 + \ln[M_2(G)]0.505\\
ct &= -57.195 + \ln[M_2(G)]102.888\\
cp &= 46.458 - \ln[M_2(G)]5.931\\
st &= 7.282 + \ln[M_2(G)]4.115\\
mp &= -195.718 + \ln[M_2(G)]28.122
\end{aligned}$$

7. Atom-Bond Connectivity index $ABC(G)$

1. Linear Model

$$\begin{aligned}
bp &= -64.716 + [ABC(G)]33.687\\
mv &= 85.034 + [ABC(G)]14.889\\
mr &= 16.060 + [ABC(G)]4.501\\
hv &= 16.908 + [ABC(G)]4.219\\
ct &= 84.789 + [ABC(G)]38.735\\
cp &= 38.675 - [ABC(G)]2.310\\
st &= 13.480 + [ABC(G)]1.445\\
mp &= -162.007 + [ABC(G)]11.401
\end{aligned}$$

2. Quadratic Model

$$\begin{aligned}
bp &= 82.424[ABC(G)]^2 - 5.262[ABC(G)] - 170.576\\
mv &= 42.667[ABC(G)]^2 - 3.003[ABC(G)] + 24.767\\
mr &= 12.555[ABC(G)]^2 - 0.871[ABC(G)] - 1.414\\
hv &= 13.605[ABC(G)]^2 - 1.015[ABC(G)] - 3.456\\
ct &= 126.152[ABC(G)]^2 - 9.438[ABC(G)] - 105.087\\
cp &= -11.102[ABC(G)]^2 + 0.949[ABC(G)] + 57.771\\
st &= 4.686[ABC(G)]^2 - 0.351[ABC(G)] + 6.452\\
mp &= 13.132[ABC(G)]^2 - 0.188[ABC(G)] - 165.747
\end{aligned}$$

3. Logarithmic Model

$$\begin{aligned}
bp &= -130.360 + \ln[ABC(G)]148.181\\
mv &= 55.600 + \ln[ABC(G)]65.736\\
mr &= 0.678 + \ln[ABC(G)]11.632\\
hv &= 8.402 + \ln[ABC(G)]18.729\\
ct &= -57.195 + \ln[ABC(G)]102.888\\
cp &= 43.926 - \ln[ABC(G)]10.623\\
st &= 10.545 + \ln[ABC(G)]6.427\\
mp &= -182.575 + \ln[ABC(G)]49.066
\end{aligned}$$

8. Augmented Zagreb Index $AZI(G)$

1. Linear Model

$$\begin{aligned} bp &= 12.424 + [AZI(G)]2.153 \\ mv &= 113.239 + [AZI(G)]1.068 \\ mr &= 24.599 + [AZI(G)]0.322 \\ hv &= 24.513 + [AZI(G)]0.311 \\ ct &= 144.923 + [AZI(G)]3.102 \\ cp &= 34.848 - [AZI(G)]0.180 \\ st &= 16.409 + [AZI(G)]0.991 \\ mp &= -134.675 + [AZI(G)]0.672 \end{aligned}$$

2. Quadratic Model

$$\begin{aligned} bp &= 7.32[AZI(G)]^2 - 0.063[AZI(G)] - 82.098 \\ mv &= 1.644[AZI(G)]^2 - 0.007[AZI(G)] + 102.697 \\ mr &= 0.526[AZI(G)]^2 - 0.002[AZI(G)] + 20.875 \\ hv &= 0.416[AZI(G)]^2 - 0.001[AZI(G)] + 22.595 \\ ct &= 7.423[AZI(G)]^2 - 0.053[AZI(G)] + 65.599 \\ cp &= -0.379[AZI(G)]^2 + 0.002[AZI(G)] + 38.502 \\ st &= 0.216[AZI(G)]^2 - 0.001[AZI(G)] + 14.281 \\ mp &= -2.142[AZI(G)]^2 - 0.035[AZI(G)] - 84.780 \end{aligned}$$

3. Logarithmic Model

$$\begin{aligned} bp &= -187.696 + \ln[AZI(G)]79.188 \\ mv &= 29.399 + \ln[AZI(G)]35.203 \\ mr &= -0.952 + \ln[AZI(G)]10.693 \\ hv &= 0.279 + \ln[AZI(G)]10.204 \\ ct &= -121.818 + \ln[AZI(G)]108.818 \\ cp &= 49.847 - \ln[AZI(G)]49.847 \\ st &= 8.076 + \ln[AZI(G)]3.142 \\ mp &= -158.803 + \ln[AZI(G)]14.474 \end{aligned}$$

9. Geometric-Airthmetic Index $GA(G)$

1. Linear Model

$$\begin{aligned} bp &= -53.490 + [GA(G)]25.569 \\ mv &= 82,145 + [GA(G)]12.497 \\ mr &= 15.201 + [GA(G)]3.777 \\ hv &= 15.556 + [GA(G)]3.624 \\ ct &= 69.372 + [GA(G)]33.814 \\ cp &= 40.776 - [GA(G)]2.201 \\ st &= 13.365 + [GA(G)]1.186 \\ mp &= -151.482 + [GA(G)]7.566 \end{aligned}$$

2. Quadratic Model

$$\begin{aligned} bp &= 84.230[GA(G)]^2 - 5.241[GA(G)] - 205.368 \\ mv &= 11.018[GA(G)]^2 + 0.132[GA(G)] + 85.974 \\ mr &= 3.426[GA(G)]^2 + 0.031[GA(G)] + 16.105 \\ hv &= 2.432[GA(G)]^2 + 0.016[GA(G)] + 18.643 \\ ct &= 64.764[GA(G)]^2 - 2.765[GA(G)] - 10.761 \\ cp &= -3.172[GA(G)]^2 + 0.087[GA(G)] + 43.297 \\ st &= 2.457[GA(G)]^2 - 0.113[GA(G)] + 10.075 \\ mp &= -16.468[GA(G)]^2 + 2.163[GA(G)] - 89.671 \end{aligned}$$

3. Logarithmic Model

$$\begin{aligned} bp &= -141.711 + \ln[GA(G)]137.672 \\ mv &= 43.969 + \ln[GA(G)]64.597 \\ mr &= 3.653 + \ln[GA(G)]19.525 \\ hv &= 4.583 + \ln[GA(G)]18.681 \\ ct &= -40.247 + \ln[GA(G)]178.218 \\ cp &= 47.764 - \ln[GA(G)]11.519 \\ st &= 9.474 + \ln[GA(G)]6.276 \\ mp &= -179.479 + \ln[GA(G)]36.726 \end{aligned}$$

10. Harmonic Index $H(G)$

1. Linear Model

$$\begin{aligned} bp &= -52.343 + [H(G)]48.668 \\ mv &= 81.662 + [H(G)]24.018 \\ mr &= 15.150 + [H(G)]7.228 \\ hv &= 15.059 + [H(G)]7.072 \\ ct &= 63.098 + [H(G)]66.687 \\ cp &= 41.516 - [H(G)]4.439 \\ st &= 13.506 + [H(G)]2.219 \\ mp &= -156.398 + [H(G)]15.763 \end{aligned}$$

2. Quadratic Model

$$\begin{aligned} bp &= 197.073[H(G)]^2 - 24.379[H(G)] - 266.711 \\ mv &= 35.395[H(G)]^2 - 1.870[H(G)] + 65.270 \\ mr &= 11.768[H(G)]^2 - 0746[H(G)] + 8.609 \\ hv &= 8.455[H(G)]^2 - 0.221[H(G)] + 13.124 \\ ct &= 186.977[H(G)]^2 - 19.760[H(G)] - 110.657 \\ cp &= -8.281[H(G)]^2 + 0.631[H(G)] + 47.065 \\ st &= 5.597[H(G)]^2 - 0.555[H(G)] + 8.644 \\ mp &= -54.423[H(G)]^2 + 11.565[H(G)] - 55.220 \end{aligned}$$

3. Logarithmic Model

$$\begin{aligned} bp &= -62.629 + \ln[H(G)]145.849 \\ mv &= 81.125 + \ln[H(G)]68.205 \\ mr &= 14.917 + \ln[H(G)]20.586 \\ hv &= 15.005 + \ln[H(G)]19.995 \\ ct &= 54.741 + \ln[H(G)]195.002 \\ cp &= 41.773 - \ln[H(G)]12.730 \\ st &= 13.276 + \ln[H(G)]64.57 \\ mp &= -150.996 + \ln[H(G)]39.806 \end{aligned}$$

11. Sum-Connectivity Index $SCI(G)$

1. Linear Model

$$\begin{aligned} bp &= -67.446 + [SCI(G)]52.484 \\ mv &= 75.934 + [SCI(G)]25.463 \\ mr &= 13.319 + [SCI(G)]7.695 \\ hv &= 13.662 + [SCI(G)]7.412 \\ ct &= 50.335 + [SCI(G)]69.578 \\ cp &= 42.146 - [SCI(G)]4.567 \\ st &= 15.125 + [SCI(G)]0.198 \\ mp &= -157.805 + [SCI(G)]16.178 \end{aligned}$$

2. Quadratic Model

$$\begin{aligned} bp &= 185.047[SCI(G)]^2 - 22.097[SCI(G)] - 254.170 \\ mv &= 22.264[SCI(G)]^2 + 0.533[SCI(G)] + 80.439 \\ mr &= 7.089[SCI(G)]^2 + 0.101[SCI(G)] + 14.172 \\ hv &= 4.756[SCI(G)]^2 + 0.442[SCI(G)] + 17.402 \\ ct &= 148.589[SCI(G)]^2 - 13.170[SCI(G)] - 60.957 \\ cp &= -7.799[SCI(G)]^2 + 0.375[SCI(G)] + 45.291 \\ st &= 0.340[SCI(G)]^2 - 0.003[SCI(G)] + 13.466 \\ mp &= -31.545[SCI(G)]^2 + 8.001[SCI(G)] - 90.965 \end{aligned}$$

3. Logarithmic Model

$$\begin{aligned} bp &= -73.005 + \ln[SCI(G)]153.008 \\ mv &= 76.842 + \ln[SCI(G)]71.244 \\ mr &= 13.577 + \ln[SCI(G)]21.543 \\ hv &= 13.999 + \ln[SCI(G)]20.678 \\ ct &= 47.812 + \ln[SCI(G)]198.806 \\ cp &= 42.171 - \ln[SCI(G)]12.932 \\ st &= 7.282 + \ln[SCI(G)]4.115 \\ mp &= -154.564 + \ln[SCI(G)]42.865 \end{aligned}$$

12. Discussion and Concluding Remarks

By inspection of the data given in tables 1 and 2, and regression equations it is possible to draw a number of conclusions for the given degree based topological indices.

- The Randic index plays an useful role in QSPR studies. The correlation coefficient value ranges from 0.073 to 0.924 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 0.086 to 0.943 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 0.065 to 0.942 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.
- The reciprocal Randic index shows less predictive power than the Randic index. The correlation coefficient value ranges from 0.082 to 0.925 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 0.082 to 0.928 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 0.081 to 0.917 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.
- The classical topological index namely the second Zagreb index shows the following applications in QSPR studies of alkanes. The correlation coefficient value ranges from 0.073 to 0.807 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 0.075 to 0.860 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 0.079 to 0.827 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.
- The atom bond connectivity index found to be useful topological index. The correlation coefficient value

ranges from 0.093 to 0.825 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for boiling point of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.093 to 0.855 with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for boiling point of alkanes respectively. Finally, for logarithmic model the correlation coefficient value ranges from 0.093 to 0.848 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for boiling point of alkanes respectively.

- The augmented Zagre index found to be less useful topological index than the *ABC*-index. The correlation coefficient value ranges from 0.049 to 0.723 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 0.088 to 0.785 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 0.761 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.

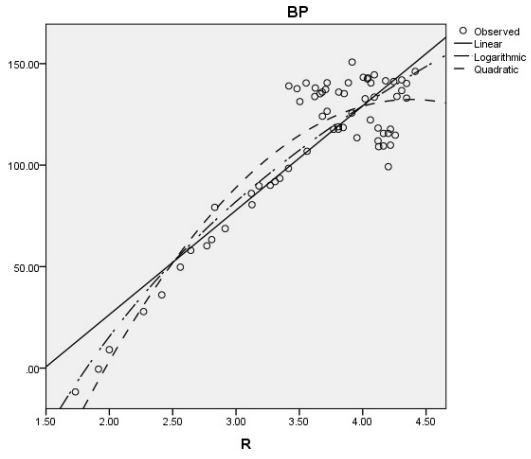
- The gometric-airthmatic index has a good predictive power for the set of alkanes. The correlation coefficient value ranges from 0.068 to 0.927 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.080 to 0.939 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 0.059 to 0.938 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.

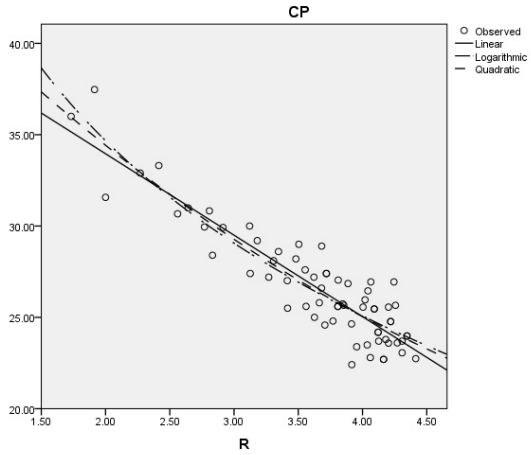
- The harmonic index has the following applications in QSPR study. The correlation coefficient value ranges from 0.070 to 0.819 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.097 to 0.870 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 0.055 to 0.857 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.

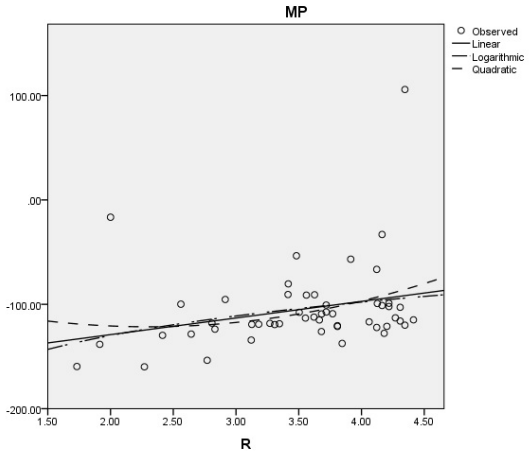
- The sum connectivity index found to be useful topological index. The correlation coefficient value ranges from 0.074 to 0.926 for linear model with minimum correlation coefficients value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively. For quadratic model the correlation coefficient value ranges from 0.066 to 0.944 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 0.084 to 0.942 with minimum correlation coefficient value for melting points of alkanes and maximum correlation coefficient value for critical temperature of alkanes respectively.

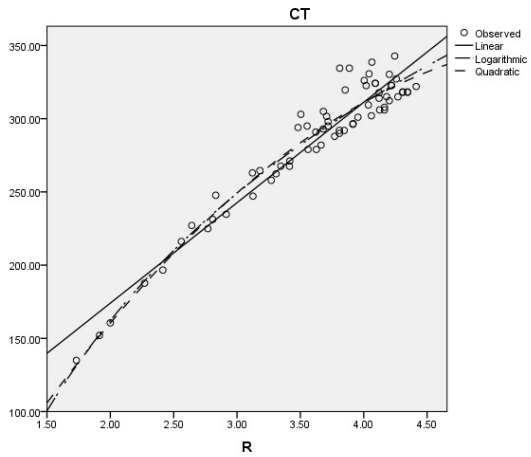
13. Correlation of Topological Indices with Physico-Chemical Properties of Alkanes

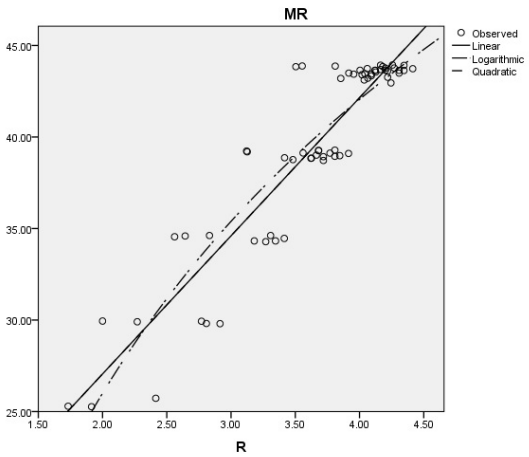
In the following figures, the correlation of topological indices with above mentioned physical properties of alkanes are shown:

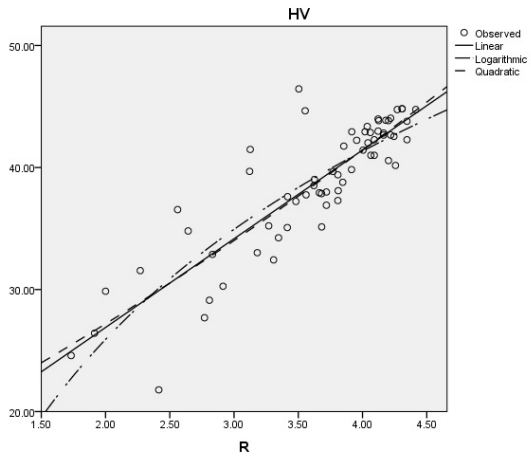


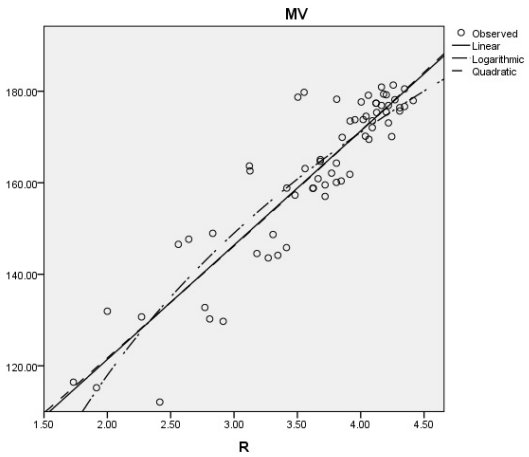

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

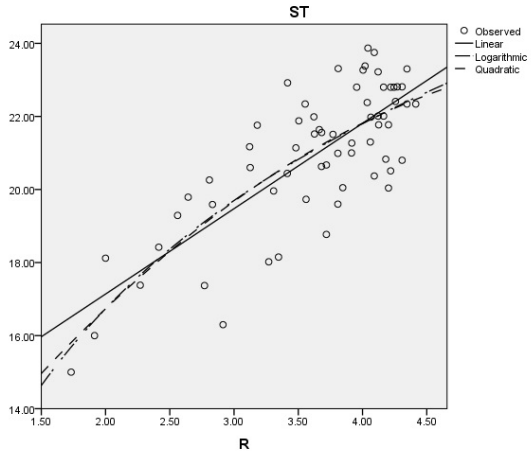

MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

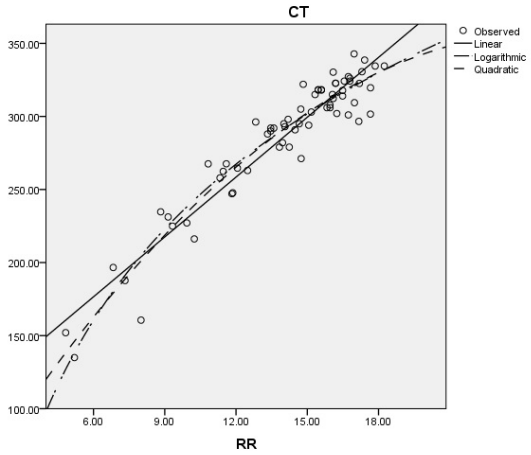

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

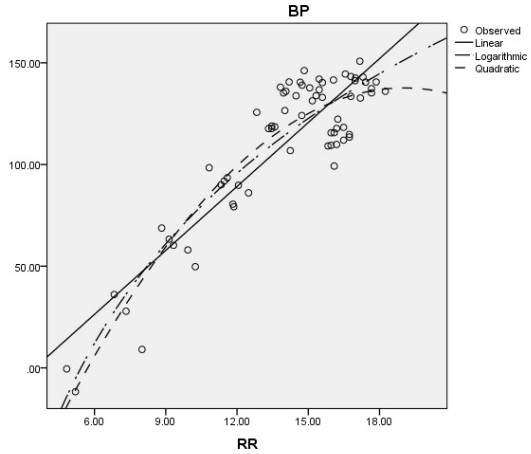

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

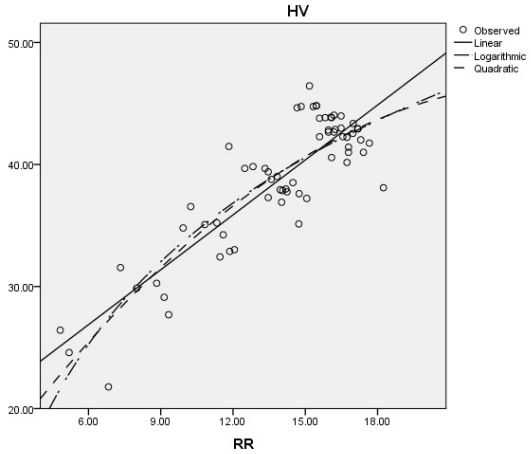

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

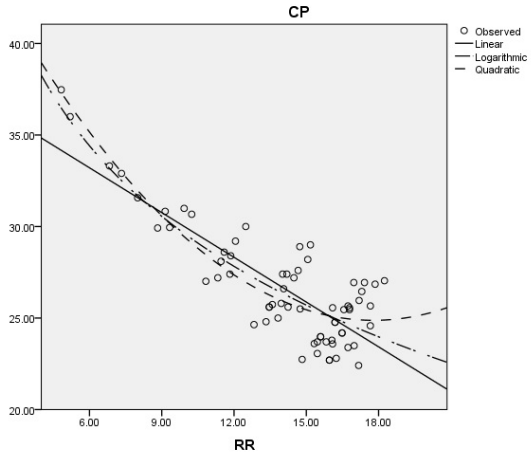

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

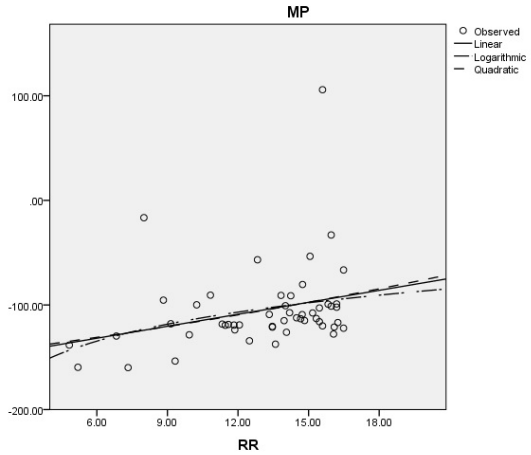

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
R

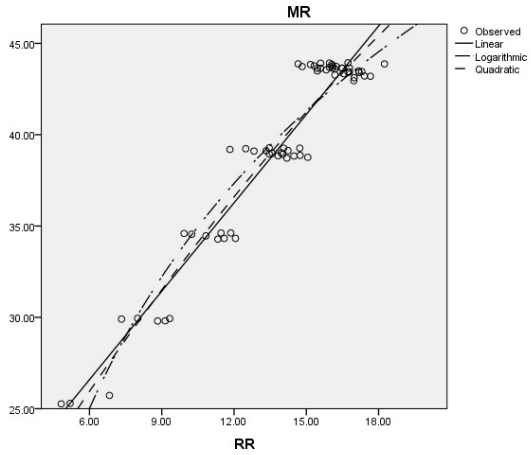

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
6.00
9.00
12.00
15.00
18.00
RR

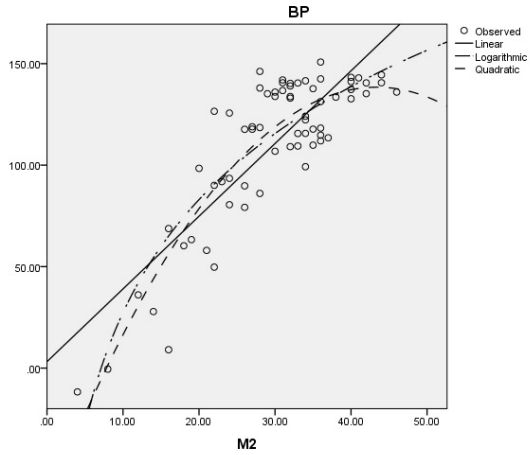

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
6.00
9.00
12.00
15.00
18.00
RR

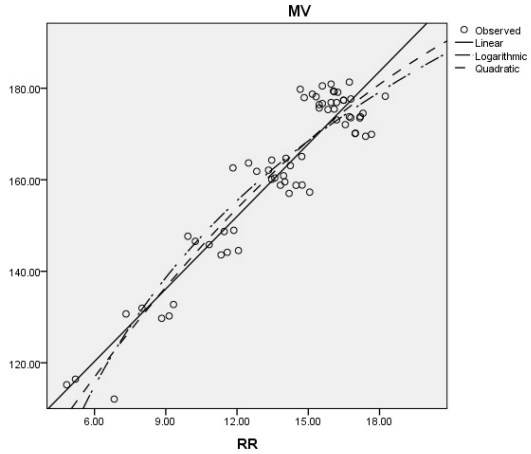

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
6.00
9.00
12.00
15.00
18.00
RR

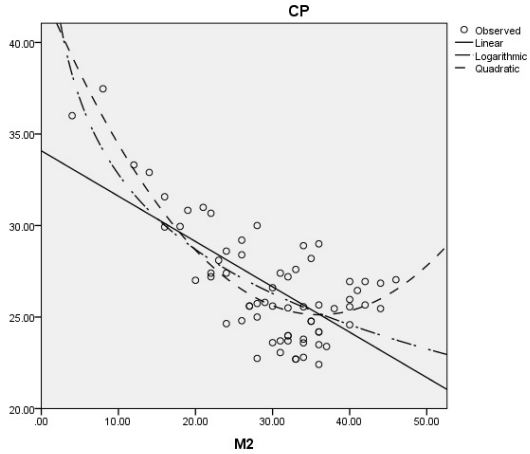

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
6.00
9.00
12.00
15.00
18.00
RR

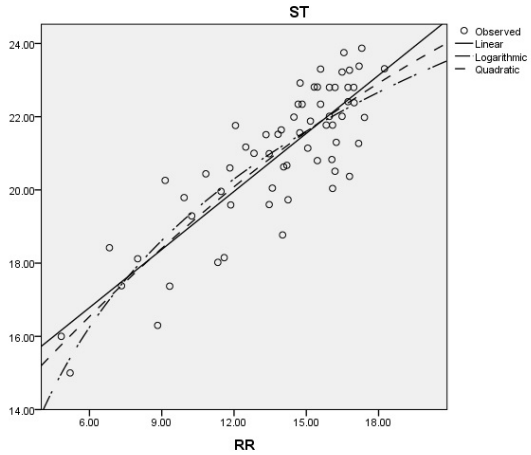

MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
6.00
9.00
12.00
15.00
18.00
RR

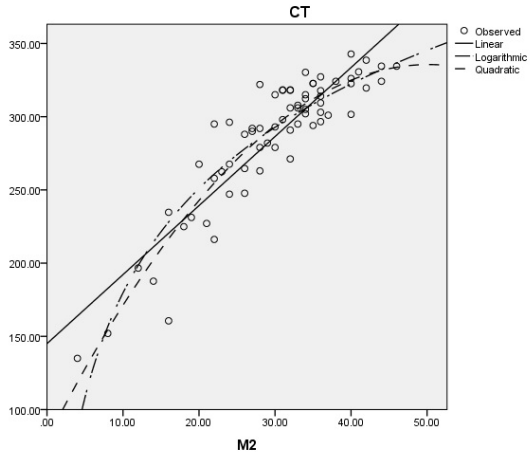

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
6.00
9.00
12.00
15.00
18.00
RR

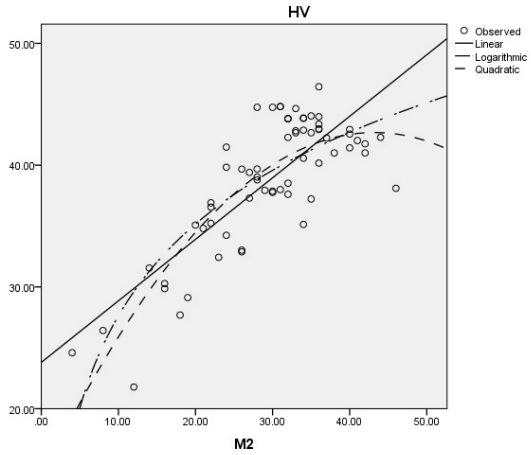

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
.00
10.00
20.00
30.00
40.00
50.00
M2

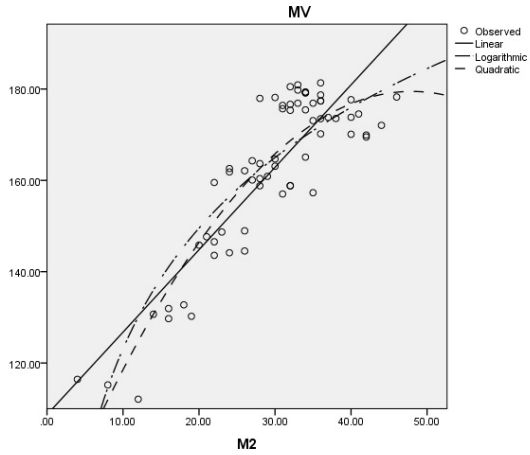

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
6.00
9.00
12.00
15.00
18.00
RR

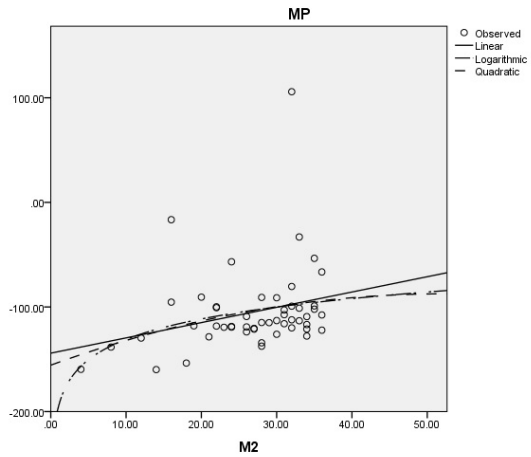

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
.00
10.00
20.00
30.00
40.00
50.00
M2

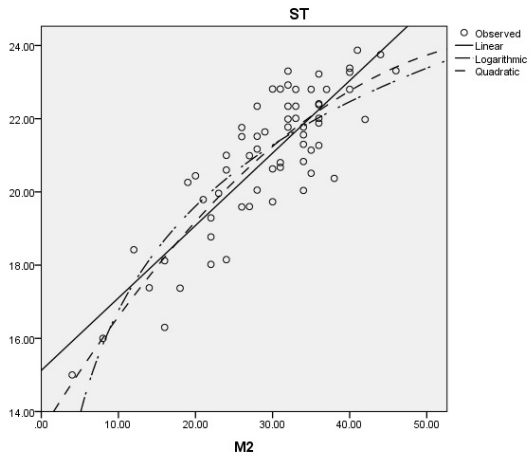

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
6.00
9.00
12.00
15.00
18.00
RR

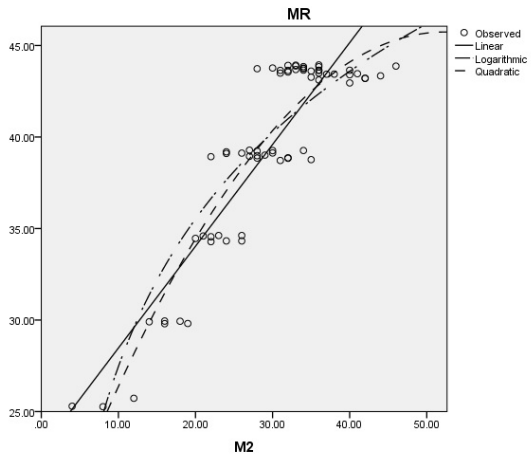

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
.00
10.00
20.00
30.00
40.00
50.00
M2

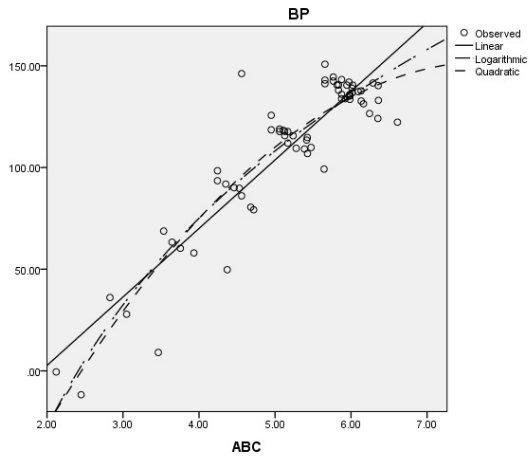

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
.00
10.00
20.00
30.00
40.00
50.00
M2

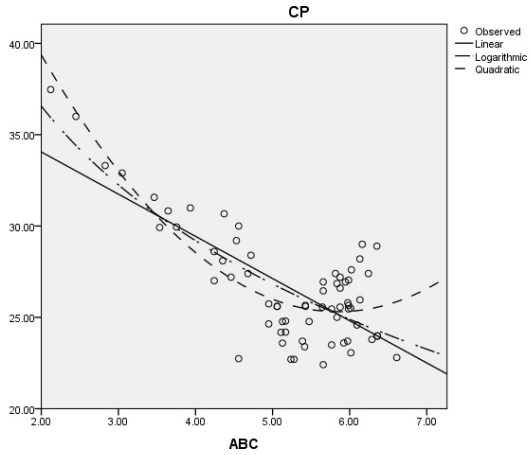

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
.00
10.00
20.00
30.00
40.00
50.00
M2

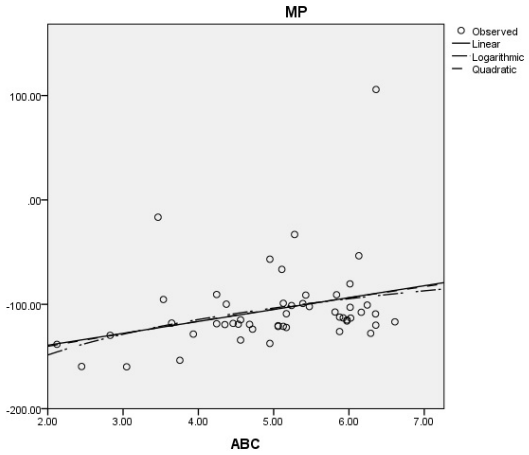

MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
.00
10.00
20.00
30.00
40.00
50.00
M2

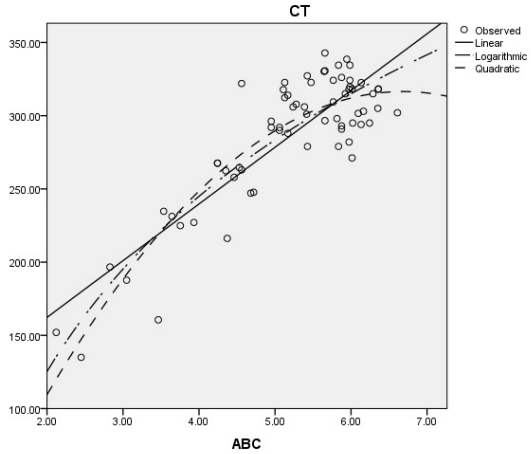

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
.00
10.00
20.00
30.00
40.00
50.00
M2

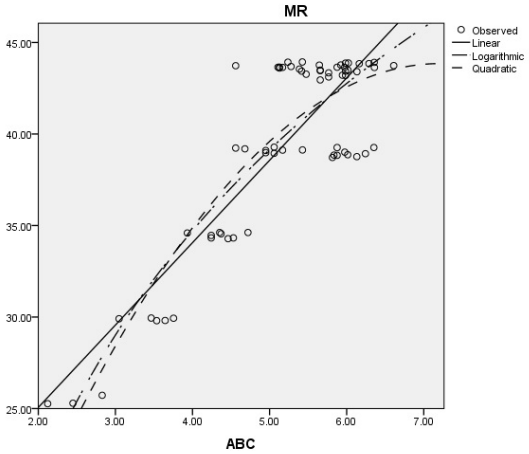

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
.00
10.00
20.00
30.00
40.00
50.00
M2

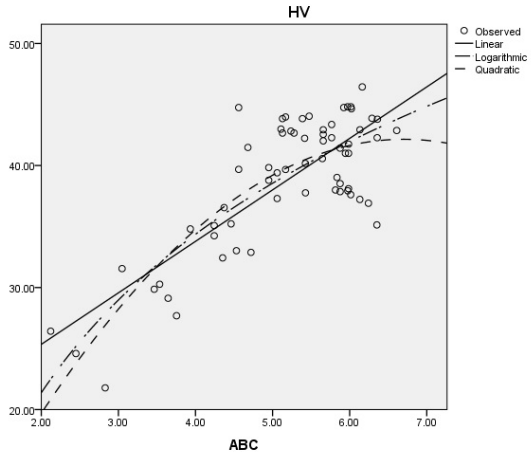

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

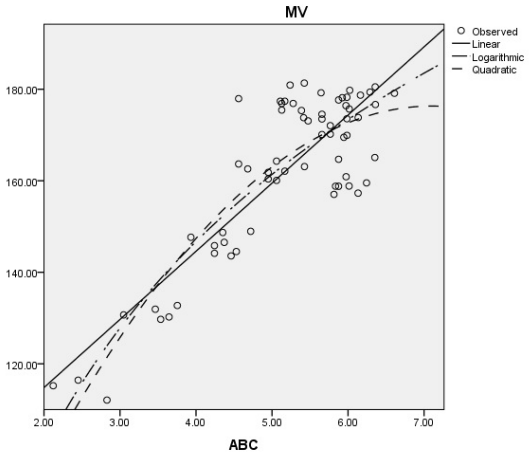

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

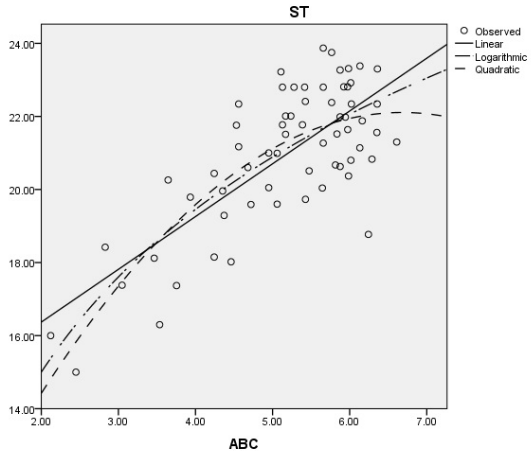

MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

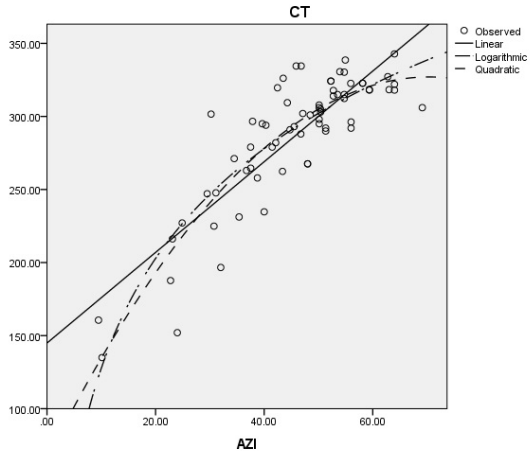

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

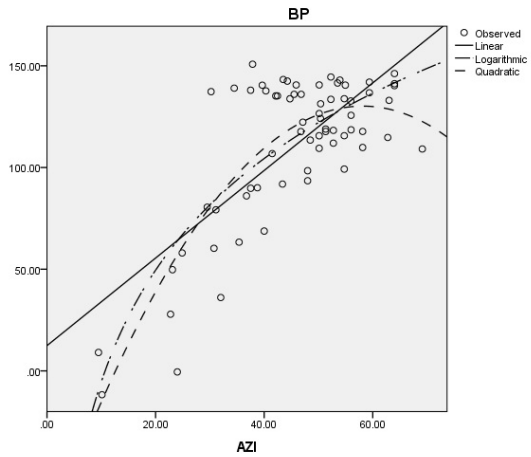

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

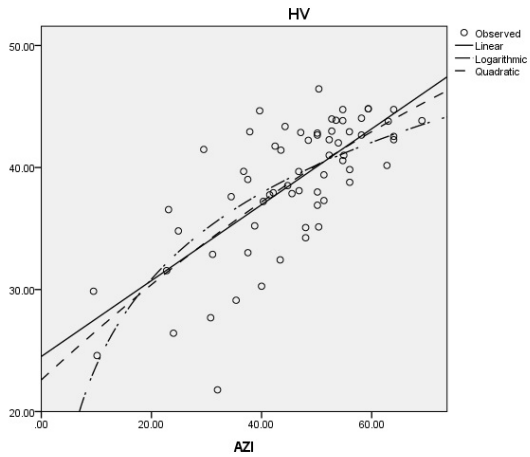

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

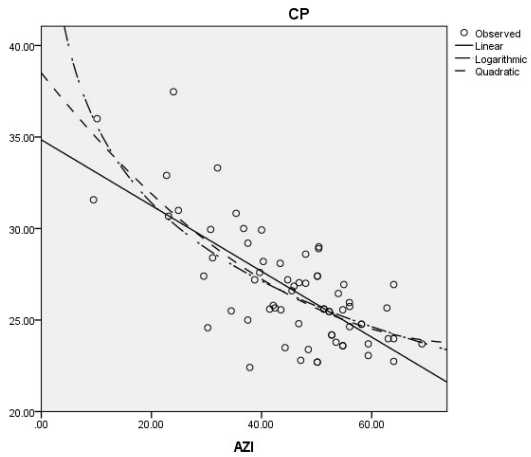

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

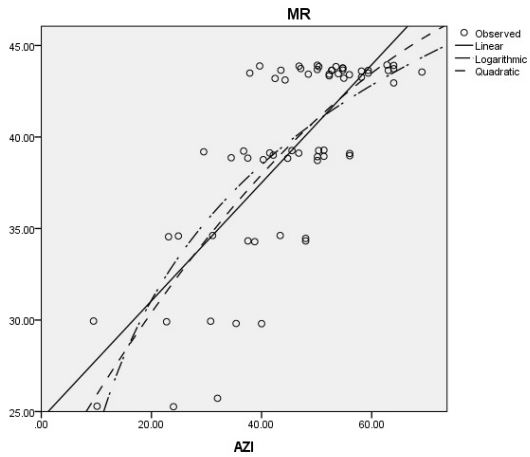

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
2.00
3.00
4.00
5.00
6.00
7.00
ABC

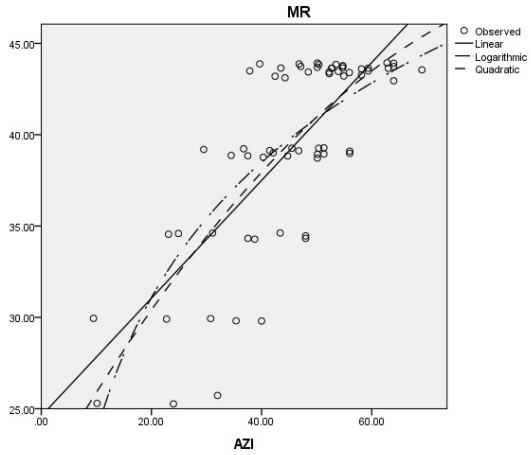

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
.00
20.00
40.00
60.00
AZI

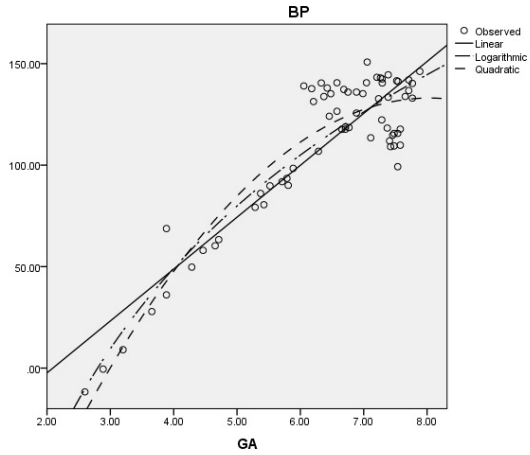

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
.00
20.00
40.00
60.00
AZI

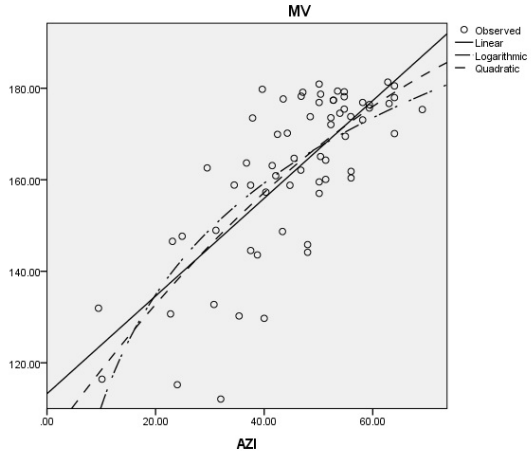

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
.00
20.00
40.00
60.00
AZI

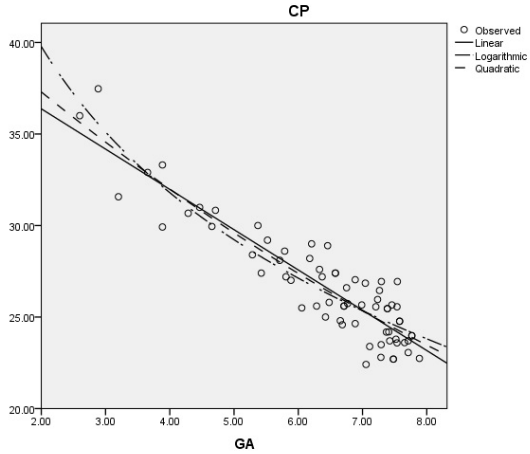

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
.00
20.00
40.00
60.00
AZI

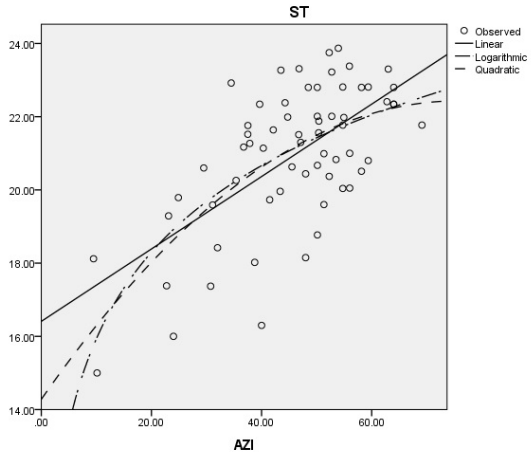

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
.00
20.00
40.00
60.00
AZI

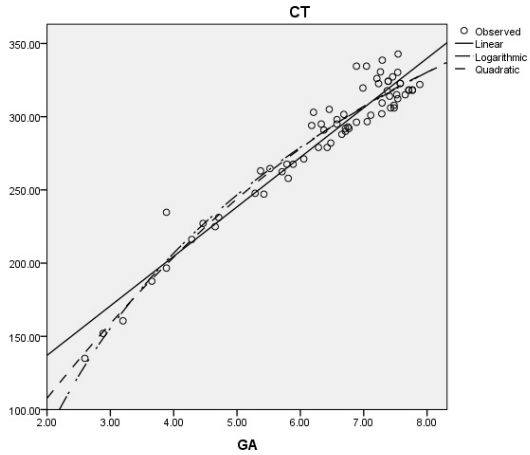

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
.00
20.00
40.00
60.00
AZI

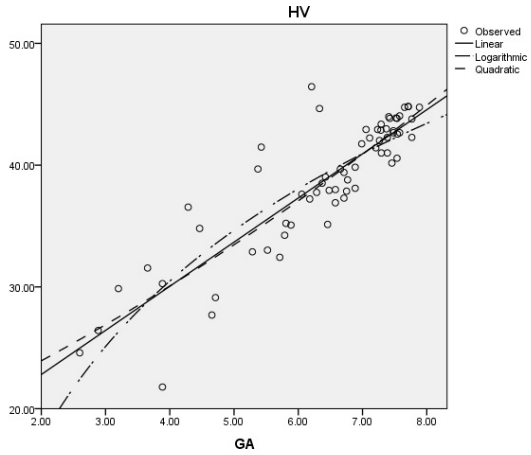

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

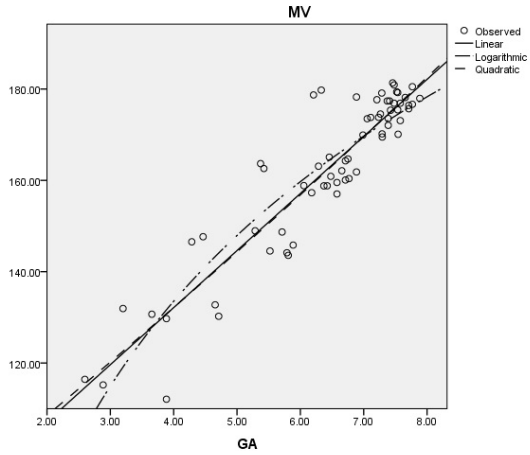

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
.00
20.00
40.00
60.00
AZI

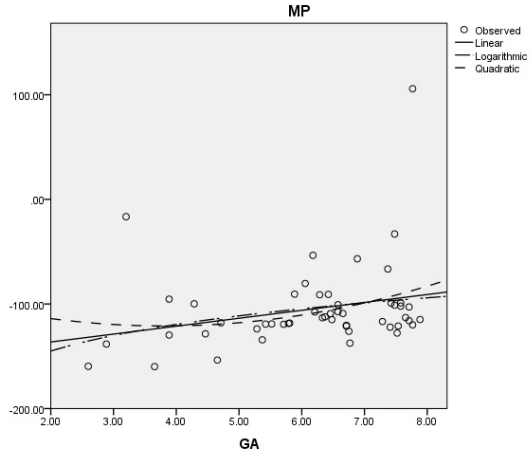

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

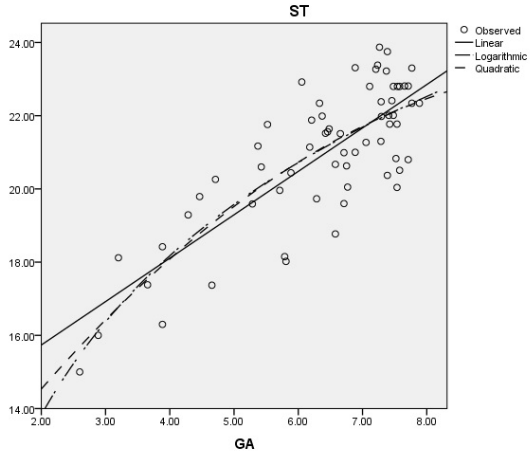

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
.00
20.00
40.00
60.00
AZI

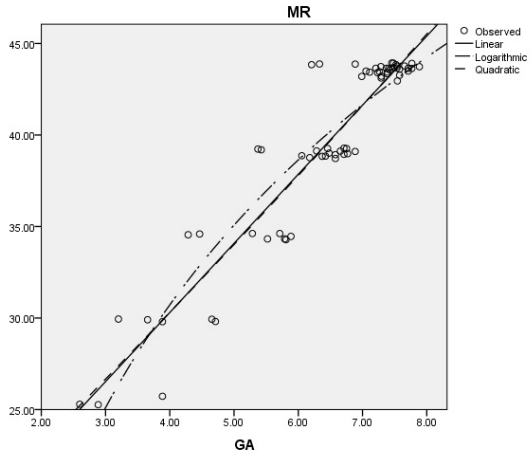

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

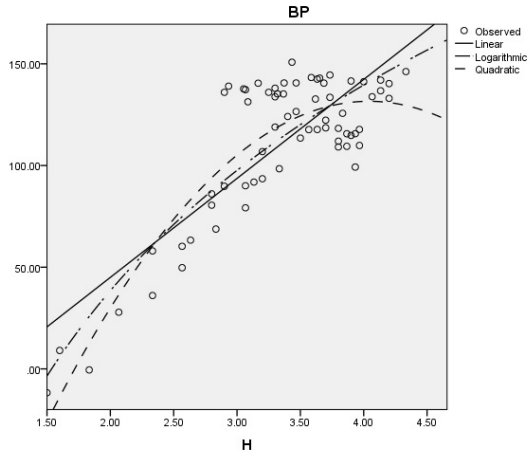

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

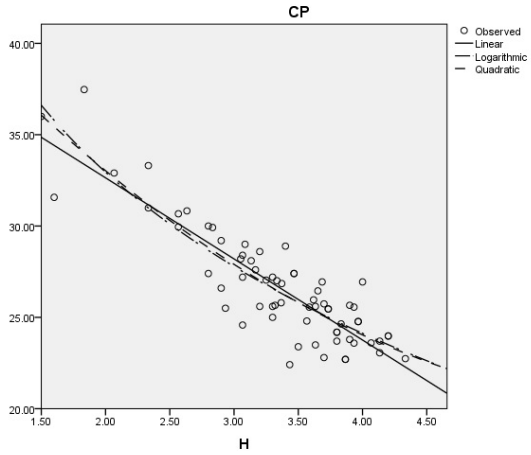

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

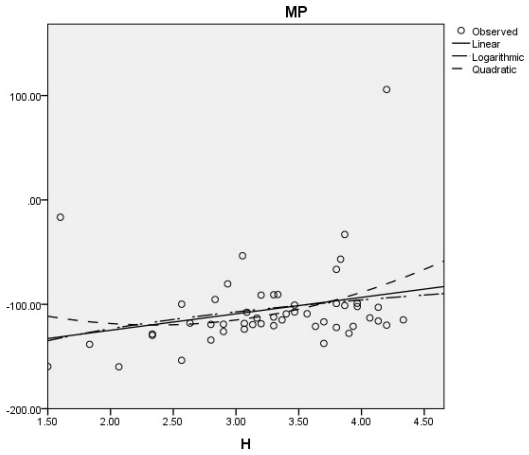

MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

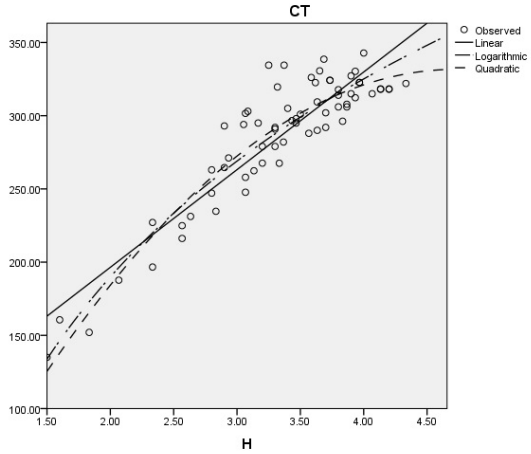

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

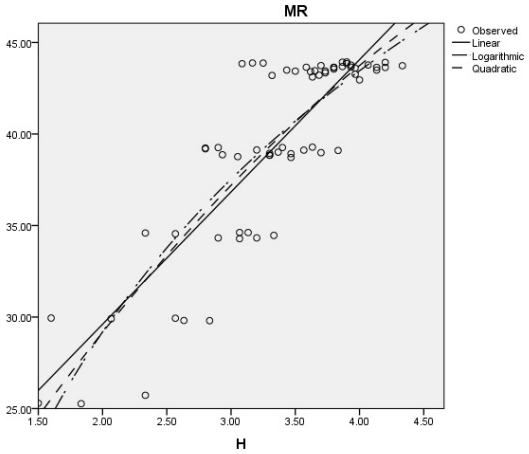

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
2.00
3.00
4.00
5.00
6.00
7.00
8.00
GA

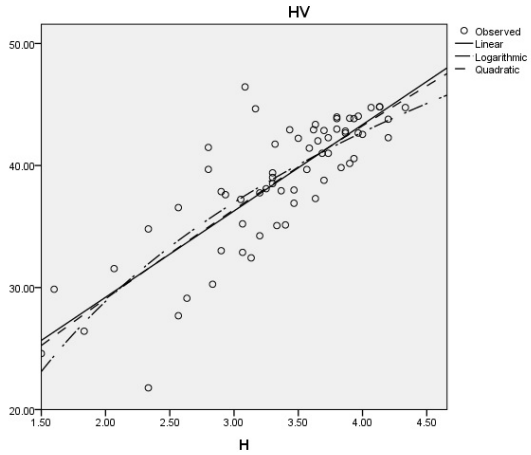

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

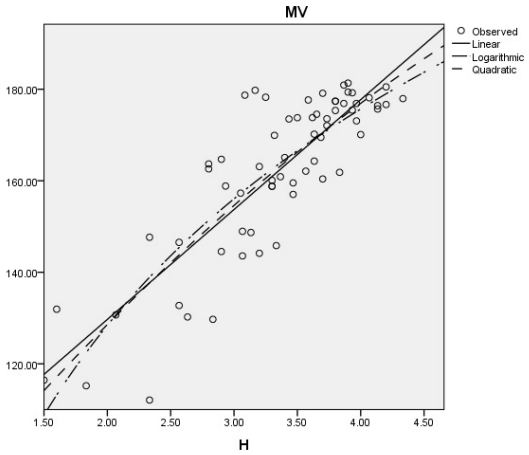

CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

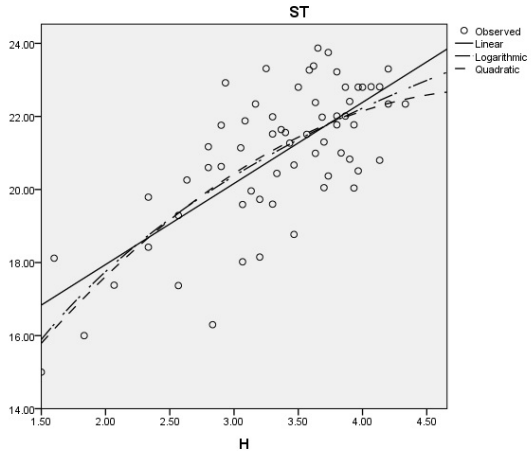

MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

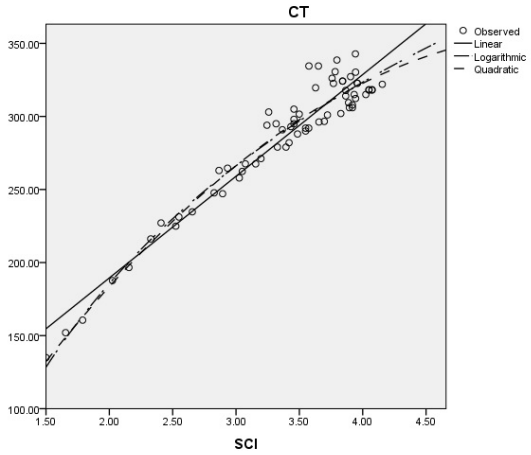

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

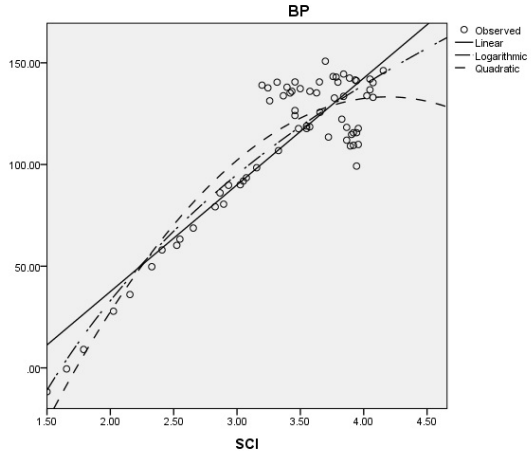

MR
Observed
Linear
Logarithmic
Quadratic
45.00
40.00
35.00
30.00
25.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

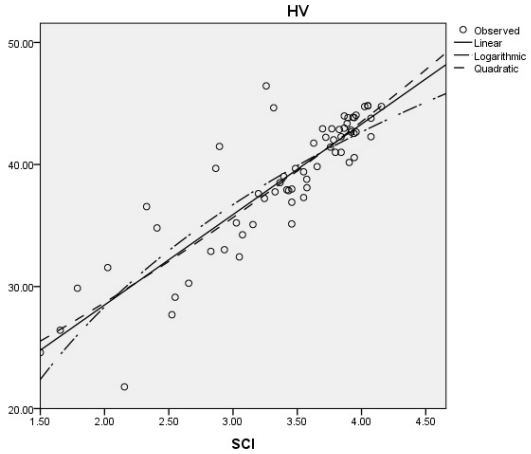

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

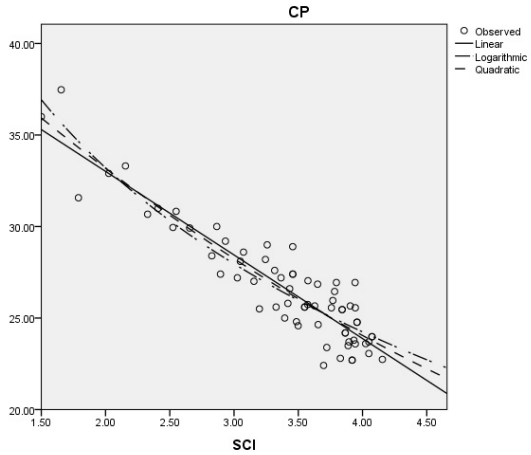

MV
Observed
Linear
Logarithmic
Quadratic
180.00
160.00
140.00
120.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

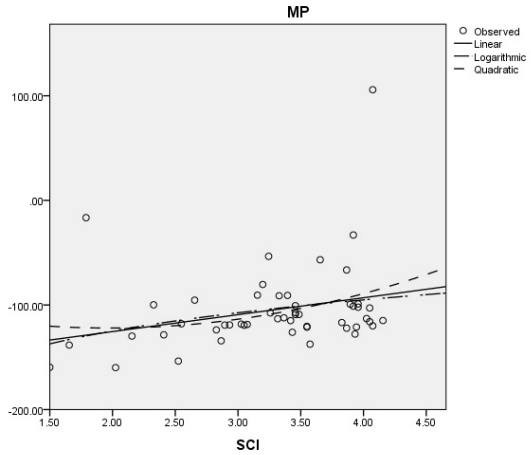

ST
Observed
Linear
Logarithmic
Quadratic
24.00
22.00
20.00
18.00
16.00
14.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
H

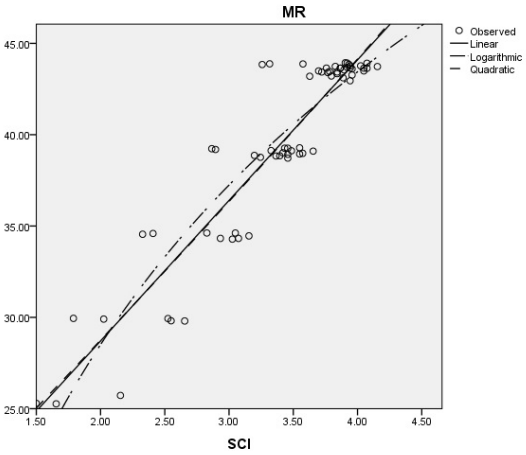

CT
Observed
Linear
Logarithmic
Quadratic
350.00
300.00
250.00
200.00
150.00
100.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
SCI

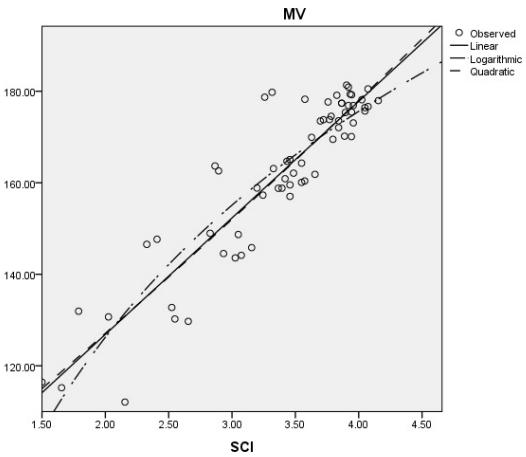

BP
Observed
Linear
Logarithmic
Quadratic
150.00
100.00
50.00
.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
SCI

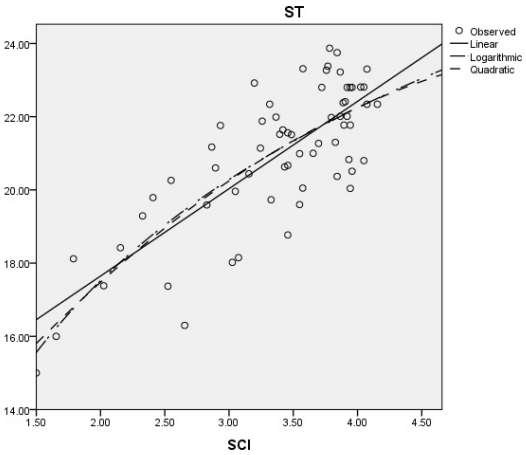

HV
Observed
Linear
Logarithmic
Quadratic
50.00
40.00
30.00
20.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
SCI


CP
Observed
Linear
Logarithmic
Quadratic
40.00
35.00
30.00
25.00
20.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
SCI


MP
Observed
Linear
Logarithmic
Quadratic
100.00
.00
-100.00
-200.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
SCI







14. Conclusion

The results of QSPR studies reveals that the regression models (3.1)-(3.3) are the most significant models to predict the physicochemical properties of molecular graphs.

15. Acknowledgment

The authors are thankful to the anonymous reviewers for their useful comments to improve the quality of the paper.

References

[1] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes. *Chemical Physics Letters*, 463(2008) 422–425.

[2] S. Fajtlowicz, Harmonic Index, *Congr. Numer.*, 60 (1987), 187–190.

[3] B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index. *Journal of Mathematical Chemistry,* 48(2010), 370–380.

[4] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.,* 17 (1972), 535–538.

[5] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta,* 86(4)(2013), 351–361.

[6] S. M. Hosamani and I. Gutman, Zagreb Indices of transformation graphs and total transformation graphs, *Appl. Math. Compt.,* 247 (2014), 1156–1160.

[7] S. M. Hosamani, B. Basavanagoud, New upper bounds for the first Zagreb index, *MATCH Commun. Math. Comput. Chem.*, 74(1)(2015), 97–101.

[8] S. M. Hosamani, S. H. Malghan and I. N. Cangul, The first geometric-arithmetic index of graph operations, *Advances and Applications in Mathematical Sciences*, 14(6)(2015), 155–163.

[9] S. M. Hosamani, Computing Sanskruti index of certain nanostructures, *J. Appl. Math. Comput*., 1-9(2016), 1209–1215.

[10] S. M. Hosamani Correlation of domination parameters with physicochemical properties of octane isomers. *Applied Mathematics and Nonlinear Sciences*, 1 (2016), 345–352.

[11] S. M. Hosamani, D. M. Perigidad, S. Y. Jamagoud, Y. B. Maled and S. Gavade, QSPR Analysis of Certain Degree Based Topological Indices, *J. Stat. Appl. Pro*., 6(2)(2017), 361–371.

[12] S. M. Hosamani, V.B. Awati and R. M. Honnamore, Estimation of numerical invariants associated with certain nanostructures and dendrimers via degree based descriptors, *Journal of Mathemaical Chemistry,* (Accepted).

[13] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc*., 97(1975), 6609–6615.

[14] D. Vukièević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, 46 (2009), 1369–1376.

[15] B. Zhou and N. Trinajstić, Sum-connectivity index, *J. Math. Chem.* 46(2009), 1252-1260.

★★★★★★★★★
ISSN(P):2319 – 3786
Malaya Journal of Matematik
ISSN(O):2321 – 5666
★★★★★★★★★