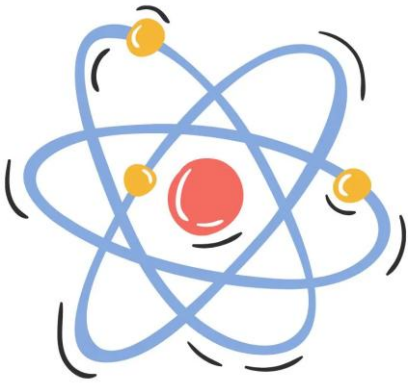


ISSN: 1672 - 6553

JOURNAL OF DYNAMICS AND CONTROL

VOLUME 10 ISSUE 02: P139-161

CURVILINEAR REGRESSION ANALYSIS OF DIABETIC DRUGS USING BANHATTI INDICES

P. Nathiya, M. Suresh

Department of Mathematics, College of Engineering and Technology,
SRM Institute of Science and Technology,
Kattankulathur 603203, Tamil Nadu. India

JOURNAL OF DYNAMICS AND CONTROL
https://doi.org/10.71058/jodac.v10i02006

CURVILINEAR REGRESSION ANALYSIS OF DIABETIC DRUGS USING BANHATTI INDICES

P. Nathiya, M. Suresh*

Department of Mathematics, College of Engineering and Technology,
SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu. India
Corresponding Author: sureshm@srmist.edu.in

Abstract: *Diabetes is a disease that arises when blood glucose (blood sugar) levels are too high. Glucose is the body's primary source of energy; the body can produce glucose, but glucose is also obtained from the foods eat. Diabetes increases the risk of vision, kidney, nerve, and heart disease. It is also linked to certain types of cancer. Taking actions to prevent or control diabetes can help reduce the chance of acquiring diabetes-related health problems. A topological index is a numerical value derived from the chemical substance's molecular structure. In this study, compute the K Banhatti indices and their multiplicative versions for each of the ten diabetes medications. Additionally, conduct a QSPR analysis using physical chemical parameters including boiling temperature, complexity, XLogP_3, and flash point.*

Keywords: *Diabetes Medications, K Banhatti indices, Molecular Structure, Physical Chemical properties and QSPR analysis.*

Introduction

Hyperglycaemia, a metabolic disorder marked by high blood sugar levels. When food is digested, glucose is released into the bloodstream to provide energy for the body. Insulin, a hormone produced by the pancreas, helps move glucose from the blood into cells in the liver, muscles, and fat for energy use. In people with diabetes, blood sugar remains high for two main reasons: either the pancreas doesn't produce enough insulin, or the body's cells become resistant to insulin, preventing them from responding to it. This results in elevated blood sugar levels [1-3]. Despite being a very diverse illness, diabetes is identified by monitoring the level of glucose, a single blood-borne chemical, regardless of the cause. Classifying diseases can become complicated, despite its practical benefits, and this might impede research and medical treatment advancements. Multiple mechanisms aimed at preventing or avoiding metabolic dysfunction work together to keep diabetes from progressing after it has already started and from causing complications. Each individual's background, predisposition to diabetes, and exposure to the environment will all influence the impact of a particular disease risk factor differently. Determining the resulting heterogeneity within diabetes through precision medicine, with regard to the risk of complications as well as the risk of diabetes, may enhance current health outcomes and open up new therapeutic options for the future[4,5].Tiwari et al.,[6] examined the statistical prevalence of the disease, evaluated the advantages and drawbacks of existing medications, and also reviewed clinical approaches in diabetology, including nanotechnology and stem cell therapies. Several factors impact the selection and management of glucose-lowering therapies, including the severity of hyperglycaemia, liver and kidney function, risks of hyperglycaemia, body mass index, the ability to self-monitor blood glucose, and the cost of medications. Treatment options for type 1 diabetes involve strategies such as enhancing islet cell survival and regeneration through islet neogenesis-associated protein (INGAP) peptide therapy, inhibiting dipeptidyl peptidase-4 (DPP-4) with medications

https://doi.org/10.71058/jodac.v10i02006

like sitagliptin, and promoting insulin release via GLP analogues such as exenatide and liraglutide, which address β-cell dysfunction[6,7].

Chemical graph theory heavily relies on topological indices. In 1947, Harold Wiener discovered the concept of topological indices and wrote the first publications elucidating the relationship between the Wiener index and the physicochemical characteristics of compounds based on carbon[8,9]. Tang JH et al.,[10] calculated various Banhatti molecular descriptors for water-soluble dendritic compounds to analyse the behaviour of water-soluble dendritic unimolecular polyether micelles as potential drug delivery agents. Numerous topological indices linked to the Wiener index were introduced in 1997.In 2016 marked the introduction of several new Banhatti indices by Indian Mathematician Kulli, including K, Modified, and Hyper-K Banhatti indices[10]. By influencing the Zagreb indices' work, Kulli introduced these indicators. Using B-indices, examined a variety of graphs, including regular, cyclic, complete, and complete bipartite graphs. Mahboob et al.,[11] analysed the specific isomer of silicon carbides using various topological indices related to vertex and edge degrees. The B-indices can be used to compare various graph operations and to characterize the characteristics of path graphs. Complex materials or substances known as nanomaterials are created and utilized to investigate the structures of various nanomaterials and well-known Jahangir graphs and studied the behaviour of linked graphs, including path, cycle, complete, and bipartite graphs, by applying the indices [11].

Ravi et al. [12] employed the reduced reverse degree-based indices to analyse a set of benzenoid hydrocarbon molecules and explored their relationship with the physicochemical properties of the selected compounds. Additionally, compared the predictive performance of the reduced reverse degree-based topological descriptors with that of 16 other existing degree-based indices. New lead compounds can be designed using topological indices based on the characteristics of currently available medications. When compared to existing drugs, these exhibit better pharmacokinetic, pharmacodynamic, and toxicological properties. This can be completed in a short amount of time with minimal computational and financial resources required. The pharmaceutical industry has driven the increasing focus on molecular descriptors due to the need to reduce costs associated with drug development and clinical trials. The creation of drugs and specialty chemicals for particular applications necessitates the development of predictive models for quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR). Accurate molecular structure representations are necessary in order to create Structure Activity Relationship (SAR) connections for pharmaceutical substances utilizing computational or theoretical methodologies. A molecular descriptor is the outcome of a logical and mathematical process that transforms chemical data, represented symbolically in a molecule, into a significant numerical value. Molecular descriptors are central to the relationships explored in quantitative structure-property (QSPR) and quantitative structure-activity (QSAR) models, with many of them being derived from topological indices. Atoms or molecules are depicted as nodes in a chemical graph, and the chemical bonds that bind them together are illustrated as links. Topological indices are molecular descriptors in graph theory. These are graph invariants with significant applications in chemistry, materials science, engineering, and pharmaceutical science. The value of a molecular descriptor is unaffected by the particular molecular representation, such as the numbering or labelling of atoms. Hydrocarbon molecules are modelled using the matching molecular graph. In this case, the edges stand in for the bonds

https://doi.org/10.71058/jodac.v10i02006

that join the carbon atoms at their vertices. The response is fascinating and d_u or d(u) indicate a vertex's degree, which is the total count of edges connected to that vertex [13,14].

Materials and Methods

Let H be a simple, connected graph with vertex set V(H) and edge set E(H). The degree $d_H(v)$ of a vertex v refers to the number of edges that are incident to v. If e = vw represents an edge in H, then both the vertex v and the edge e are incident, denoted as ve. The degree of an edge e in H, denoted by $d_H(e)$,is given by the formula $d_H(e) = d_H(v) + d_H(w) - 2$ where e = vw[15,16].

Definition 1: The first K Banhatti index of a graph H is defined as[17]

$$B_1(H) = \sum_{ve}[d_H(v) + d_H(e)]$$

Definition 2: The first K hyper Banhatti index of a graph H is defined as[18]

$$HB_1(H) = \sum_{ve}[d_H(v) + d_H(e)]^2$$

Definition 3: The second K Banhatti index of a graph H is defined as[17]

$$B_2(H) = \sum_{ve}[d_H(v)\, d_H(e)]$$

Definition 4: The second K hyper Banhatti index of a graph H is defined as[18]

$$HB_2(H) = \sum_{ve}[d_H(v)\, d_H(e)]^2$$

Definition 5: The K Banhatti harmonic index of a graph H is defined as[19]

$$H_b(H) = \sum_{ve}\frac{2}{[d_H(v) + d_H(e)]}$$

Definition 6: The first multiplicative K Banhatti index of a graph H is proposed as[19]

$$BII_1(H) = \prod_{ve}[d_H(v) + d_H(e)]$$

Definition 7: The first multiplicative K hyper Banhatti index of a graph H is defined as[19]

$$HBII_1(H) = \prod_{ve}[d_H(v) + d_H(e)]^2$$

Definition 8: The second multiplicative K Banhatti index of a graph H is proposed as[19]

$$BII_2(H) = \prod_{ve}[d_H(v)\, d_H(e)]$$

Definition 9: The second multiplicative K hyper Banhatti index of a graph H is proposed as[19]

$$HBII_2(H) = \prod_{ve}[d_H(v)\, d_H(e)]^2$$

Definition 10: The K Banhatti multiplicative harmonic index of a graph H is defined as[19]

$$HII_b(H) = \prod_{ve}\frac{2}{[d_H(v) + d_H(e)]}$$

Results and Discussions

The ten diabetes medications – Tolazamide (α_1), Dapagliflozin (α_2), Miglitol (α_3), Glibenclamide (α_4), Metformin (α_5), Alogliptin (α_6), Tolbutamide (α_7), Nateglinide (α_8), Repaglinide (α_9), and Linagliptin (α_{10}) are modelled using ten Banhatti indices in this section of the model. The values for these attributes were obtained using Chemspider. Fig.1 to Fig.10

https://doi.org/10.71058/jodac.v10i02006

display the chemical structures of ten various medications. The previously mentioned degree-based edge partition of the medications is presented in Tables 1-10.

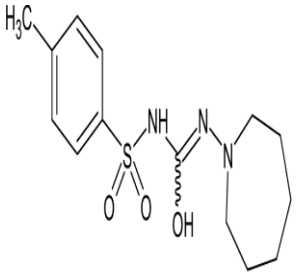


Figure 1: α_1- molecular structure

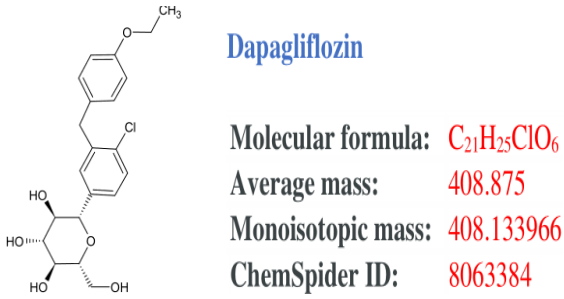


Figure 2: α_2- molecular structure

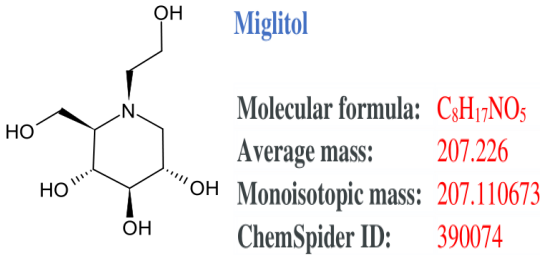


Figure 3: α_3- molecular structure

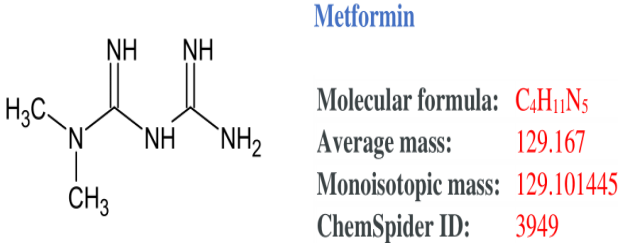


Figure 4: α_4- molecular structure

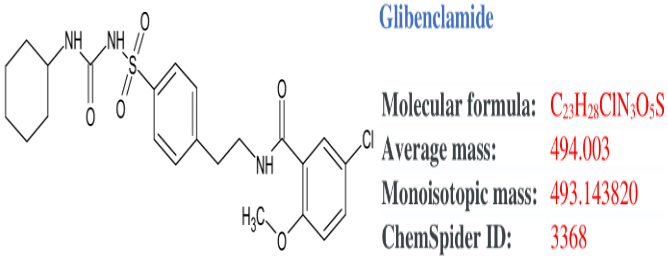


Figure 5: α_5- molecular structure

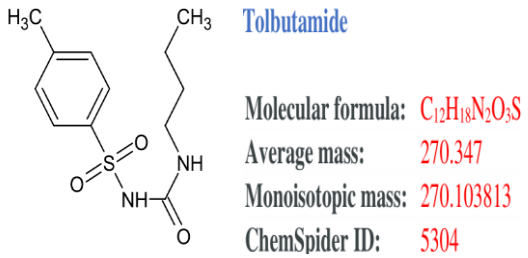


Figure 6: α_6- molecular structure

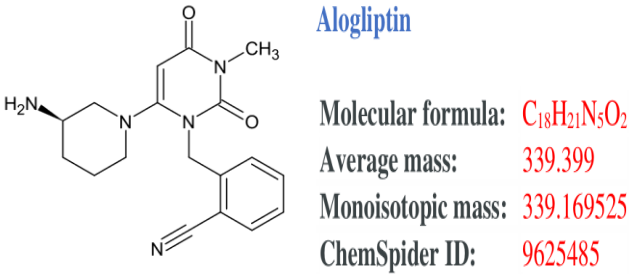


Figure 7: α_7- molecular structure

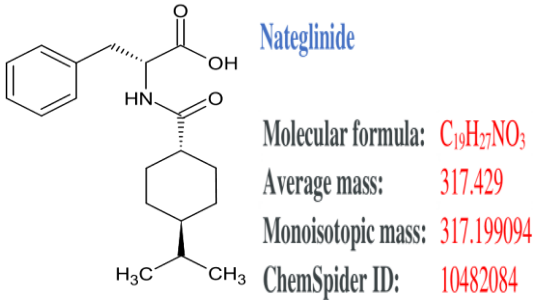
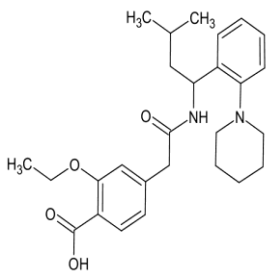


Figure 8: α_8- molecular structure

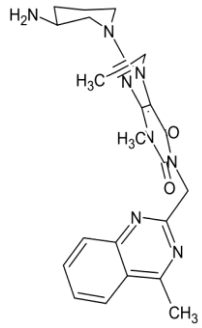
https://doi.org/10.71058/jodac.v10i02006



Repaglinide

Molecular formula: $C_{27}H_{36}N_2O_4$
Average mass: 452.595
Monoisotopic mass: 452.267508
ChemSpider ID: 4388

Figure 9 : α_9- molecular structure



Linagliptin

Molecular formula: $C_{25}H_{28}N_8O_2$
Average mass: 472.553
Monoisotopic mass: 472.233522
ChemSpider ID: 22376247

Figure 10: α_{10}- molecular structure

Table 1. Tolazamide Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(2,2)	(1,4)	(3,2)	(2,4)	(3,4)
$d_H(e)$	2	2	3	3	4	5
No. of Edges	2	7	2	9	1	1

Table 2. Dapagliflozin Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(1,2)	(2,2)	(3,2)	(3,3)
$d_H(e)$	2	1	2	3	4
No. of Edges	4	2	4	14	6

Table 3. Miglitol Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(1,2)	(3,3)	(3,2)	(2,2)
$d_H(e)$	2	1	4	3	2
No. of Edges	3	2	4	4	1

Table 4. Glibenclamide Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)	(2,4)	(3,3)	(3,4)
$d_H(e)$	1	2	3	2	3	4	4	5
No.of Edges	1	3	2	9	16	1	2	1

Table 5. Metformin Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(2,3)	(3,3)
$d_H(e)$	2	3	4
No. of Edges	5	2	1

https://doi.org/10.71058/jodac.v10i02006

Table 6. Alogliptin Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(2,3)	(2,2)	(3,3)
$d_H(e)$	2	3	2	4
No. of Edges	5	10	5	6

Table 7. Tolbutamide Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(1,2)	(1,4)	(2,2)	(2,3)	(2,4)	(3,4)
$d_H(e)$	2	1	3	2	3	4	5
No. of Edges	2	1	2	5	6	1	1

Table 8. Nateglinide Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(2,2)	(2,3)	(3,3)
$d_H(e)$	2	2	3	4
No. of Edges	5	6	10	3

Table 9. Repaglinide Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,3)	(1,2)	(2,2)	(2,3)	(3,3)
$d_H(e)$	2	1	2	3	4
No. of Edges	4	2	9	16	5

Table 10. Linagliptin Degree-based edge partitioning.

$d_H(v),d_H(w)$	(1,2)	(1,3)	(2,3)	(3,3)	(2,2)
$d_H(e)$	1	2	3	4	2
No. of Edges	1	4	17	9	5

https://doi.org/10.71058/jodac.v10i02006

Table 11. displays the values of Physicochemical properties of medications used in Diabetic treatment.

Medications	$BP(℃)$	Complexity(bit)	$XLogP_3$	FP
Tolazamide	484.5	431	1.5	246.8
Dapagliflozin	609	472	2.3	322.1
Miglitol	453.7	179	-2.6	284.3
Glibenclamide	705.7	746	4.8	380.6
Metformin	172.5	132	-1.3	58.1
Alogliptin	519.2	622	0.6	261.8
Tolbutamide	430	354	2.3	213.9
Nateglinide	527.6	393	3.2	272.9
Repaglinide	672.9	619	5.2	360.8
Linagliptin	661.2	885	1.9	353.7

Table 12. The acquired topological index values of Banhatti indices for the Diabetic treatment

Medications	$B_1(H)$	$HB_1(H)$	$B_2(H)$	$HB_2(H)$	$H_b(H)$	$BII_1(H)$	$HBII_1(H)$	$BII_2(H)$	$HBII_2(H)$	$HII_b(H)$
α_1	224	1216	297	2608	22.8	3.22E+30	1.04E+61	7.51E+33	5.64E+67	5.64E-18
α_2	312	1732	424	3664	25.28	7.91E+41	6.25E+83	8.69E+46	7.55E+93	1.46E-24
α_3	142	796	192	4662	12.7	9.08E+18	8.24E+37	4.04E+20	1.63E+41	2.96E-11
α_4	358	1950	476	4112	29.36	3.9E+48	1.52E+97	1.28E+54	1.6E+108	3.03E-28
α_5	76	390	94	722	7.4	3.35E+10	1.12E+21	1.04E+11	1.09E+22	1.96E-06
α_6	274	1528	374	3258	21.1	6.51E+36	4.24E+73	4.9E+41	2.41E+83	6.92E-22
α_7	180	982	238	2198	15.9	2.8E+24	7.82E+48	3.73E+26	1.39E+53	2.46E-14
α_8	240	1266	310	2426	20.38	8.85E+32	7.83E+65	2.63E+36	6.91E+72	3.18E-19
α_9	360	1916	470	3770	31.19	1.52E+49	2.32E+98	1.84E+54	3.4E+108	3.1E-28
α_{10}	390	2228	546	4906	28.54	6.7E+51	4.5E+103	3.27E+59	1.1E+119	7.05E-31

https://doi.org/10.71058/jodac.v10i02006

Regression models

The most reliable approximation of the relationship between topological indices and physical and chemical properties of diabetic medicines was identified using three different regression models.

$$P = \varphi_1(TI) + \epsilon, \quad \text{(Linear)} \quad (1)$$

$$P = \varphi_2(TI)^2 + \varphi_1(TI) + \epsilon, \quad \text{(Quadratic)} \quad (2)$$

$$P = \varphi_1 + \epsilon\, ln\,(TI), \quad \text{(Logarithmic)} \quad (3)$$

where P stands for physical attribute, TI stands for the topological index, φ_i and ϵ are constants.

Logarithmic, quadratic, and linear models are fitted to the curves using regression models. Here, a couple of the best topological index regression model predictors for this particular physicochemical characteristic are highlighted. The regression model list the best to test and utilize in this investigation as a consequence. Regression models were employed to fit curves instead of straight lines[20-23]. After modifying and examining the models for the physicochemical properties such as Boiling point, Complexity, $XLogP_3$ and Flash point provided in Table 11 with respect to each of the prescribed Banhatti indices outlined in Table 12, the subsequent findings were observed for the linear and quadratic regression models respectively. Topological indices with $R^2 \geq 0.8$ were taken into consideration in accordance with the International Academy of Mathematical Chemistry's (IAMC) standards[24-26].

Table.13 identifies the best predictors from Linear regression model.

Property	Predictors	R^2	Best Predictors
BP	$B_1(H)$	**0.892**	$B_1(H)$
	$HB_1(H)$	0.880	-
	$B_2(H)$	0.878	-
	$H_b(H)$	**0.892**	$H_b(H)$
Complexity	$B_1(H)$	0.884	-
	$HB_1(H)$	**0.902**	$HB_1(H)$
	$B_2(H)$	0.901	-

The bolded values shows the high correlation between physical characteristics of medications and Banhatti indices.

According to the linear regression model, only two properties can be predicted by the recommended indices which are shown in Table.13. Boiling point can be predicted by the two Banhatti indices namely $B_1(H)$ and $H_b(H)$, Complexity can be predicted by $HB_1(H)$ and $B_2(H)$. As per the quadratic regression model, in the Table 14 see that the properties Boiling point, Complexity and Flash point can be predicted by $HB_1(H)$, $HB_1(H)$ and $B_2(H)$, $HB_2(H)$ respectively. Further, for the logarithmic model, listed in Table 15,the majority of indices are correlated with the physical-chemical properties. The three different models are unable to forecast the same attribute, XLogP3, using the Banhatti indices.[26-28]

https://doi.org/10.71058/jodac.v10i02006

Table.14 identifies the best predictors from Quadratic regression model.

Property	Predictors	R^2	Best Predictors
BP	$B_1(H)$	0.923	-
	$HB_1(H)$	**0.926**	$HB_1(H)$
	$B_2(H)$	0.923	-
	$H_b(H)$	0.907	-
Complexity	$B_1(H)$	0.891	-
	$HB_1(H)$	**0.910**	$HB_1(H)$
	$B_2(H)$	**0.910**	$B_2(H)$
FP	$B_1(H)$	0.804	-
	$HB_1(H)$	0.815	-
	$B_2(H)$	0.812	-
	$HB_2(H)$	**0.878**	$HB_2(H)$

The bolded values shows the high correlation between physical characteristics of medications and Banhatti indices.

Table.15 identifies the best predictors from Logarithmic regression model.

Property	Predictors	R^2	Best Predictors
BP	$B_1(H)$	**0.937**	$B_1(H)$
	$HB_1(H)$	**0.937**	$HB_1(H)$
	$B_2(H)$	0.936	-
	$H_b(H)$	0.918	-
	$BII_1(H)$	0.895	-
	$HBII_1(H)$	0.895	-
	$BII_2(H)$	0.885	-
	$HBII_2(H)$	0.885	-
	$HII_b(H)$	0.886	-
Complexity	$B_1(H)$	0.800	-
	$HB_1(H)$	0.802	-
	$B_2(H)$	0.802	-
	$BII_1(H)$	0.876	-
	$HBII_1(H)$	0.876	-
	$BII_2(H)$	**0.891**	$BII_2(H)$
	$HBII_2(H)$	**0.891**	$HBII_2(H)$
	$HII_b(H)$	**0.891**	$HII_b(H)$
FP	$B_1(H)$	0.832	-
	$HB_1(H)$	0.842	-
	$B_2(H)$	0.840	-
	$HB_2(H)$	**0.859**	$HB_2(H)$

The bolded values shows the high correlation between physical characteristics of medications and Banhatti indices.

https://doi.org/10.71058/jodac.v10i02006

The quadratic regression models created for the physical attributes, as shown in Table 14, reveal that the quadratic regression results in the following models, which utilize B1(H) to predict the boiling point, complexity, and flash point.

$$BP = 18.041(B_1(H))^2 + 2.820(B_1(H)) - 0.002 \quad (4)$$

$$COM = 29.533(B_1(H))^2 + 1.141(B_1(H)) + 0.002 \quad (5)$$

$$FP = -10.055(B_1(H))^2 + 1.609(B_1(H)) - 0.001 \quad (6)$$

The following is a description of the quadratic regression models that use $HB_1(H)$ for predicting boiling point, complexity and flash point:

$$BP = 11.881(HB_1(H))^2 + 0.536(HB_1(H)) - 0.000 \quad (7)$$

$$COM = 36.098(HB_1(H))^2 + 0.205(HB_1(H)) + 7.04E\text{-}05 \quad (8)$$

$$FP = -17.034(HB_1(H))^2 + 0.311(HB_1(H)) - 6.4E\text{-}05 \quad (9)$$

The quadratic regression models using $B_2(H)$ that are employed to forecast the physical attributes such as boiling point, complexity and flash point:

$$BP = 18.072(B_2(H))^2 + 2.171(B_2(H)) - 0.001 \quad (10)$$

$$COM = 37.640\ (B_2(H))^2 + 0.849(B_2(H)) + 0.001 \quad (11)$$

$$FP = -12.811(B_2(H))^2 + 1.256(B_2(H)) - 0.001 \quad (12)$$

The following outcome of the quadratic regression models that use $H_b(H)$ for anticipating boiling point:

$$BP = -5.391(H_b(H))^2 + 32.933(H_b(H)) - 0.346 \quad (13)$$

The quadratic regression models, which make use of $HB_2(H)$, for assessing the flash point:

$$FP = -61.345(HB_2(H))^2 + 0.172(HB_2(H)) - 1.9E\text{-}05 \quad (14)$$

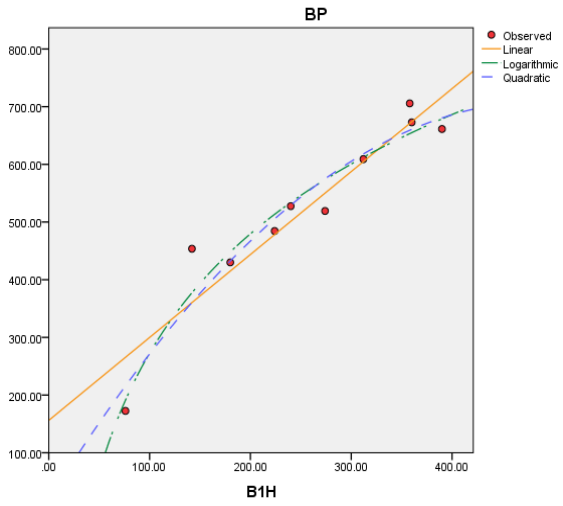


Figure 11a.Boiling point on $B_1(H)$

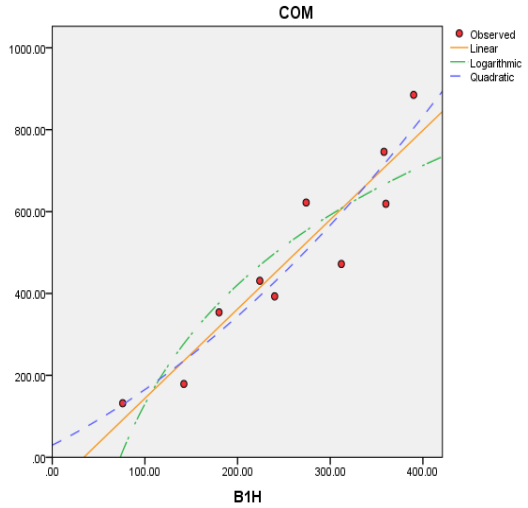


Figure 11b.Complexity on $B_1(H)$

https://doi.org/10.71058/jodac.v10i02006

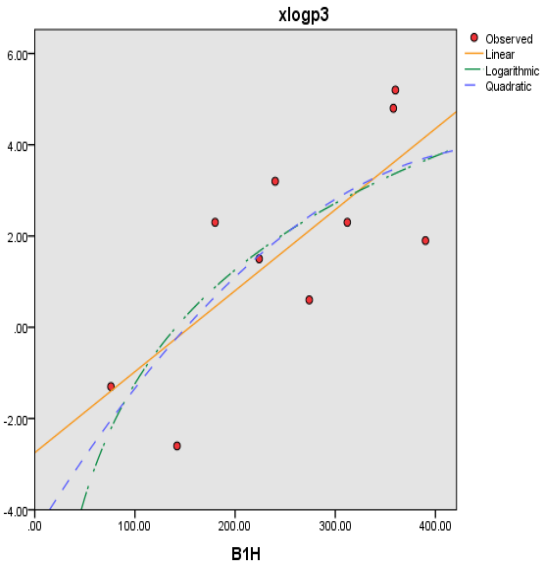


Figure 11c.XLogP$_3$ on B$_1$(H)

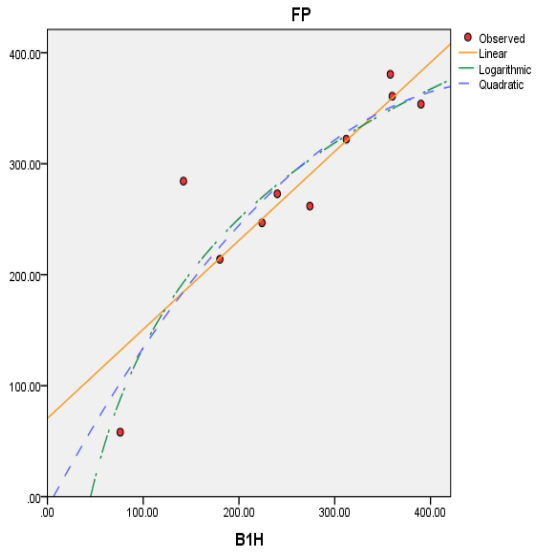


Figure 11d.Flash point on B$_1$(H)

Figure 11. Visual representations of the B$_1$(H) regression analysis.

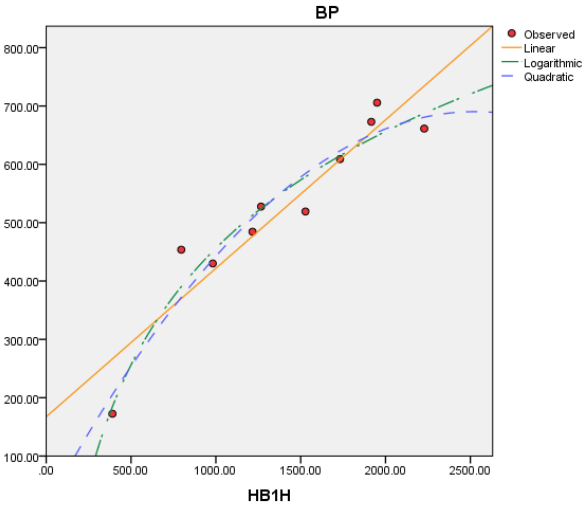


Figure 12a.Boiling point on HB$_1$(H)

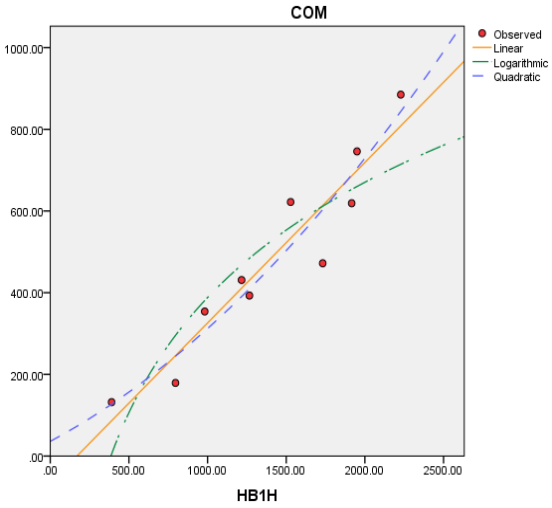


Figure 12b.Complexity on HB$_1$(H)

https://doi.org/10.71058/jodac.v10i02006

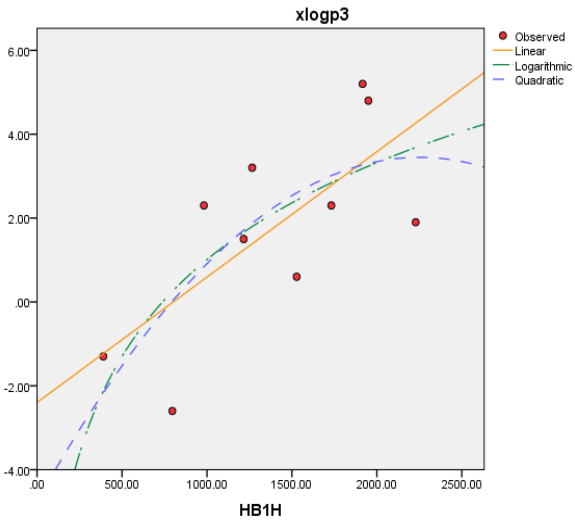


Figure 12c.XLogP$_3$ on HB$_1$(H)

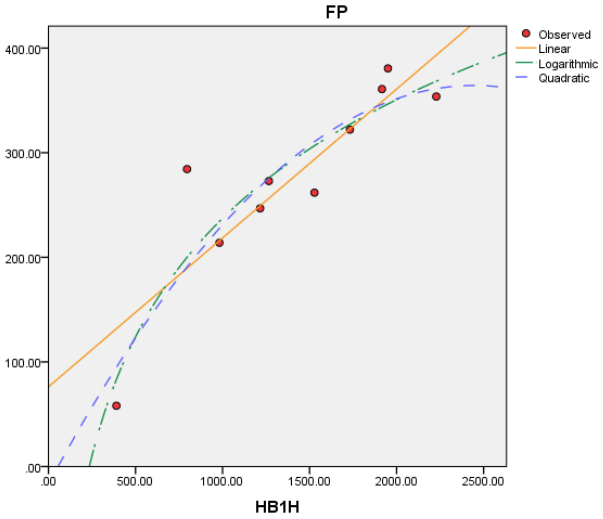


Figure 12d.Flash point on HB$_1$(H)

Figure 12. Visual representations of the HB$_1$(H) regression analysis.

Based on the quadratic regression models, the multiplicative K Banhatti indices cannot be the best predictors. In particular the quadratic model could not be fitted due to near collinearity among model terms for the multiplicative Banhatti indices BII$_2$(H), BII$_1$(H) and HII$_b$(H).

Next shows the logarithmic regression models that were created based on the indices listed in Table 15 for the physical qualities. According to the data, the logarithmic regression creates the following models, which employ B$_1$(H) to predict boiling point, complexity, and flash point:

$$BP = -1101.09 + 298.32\ ln(B_1(H)) \quad (15)$$

$$COM = -1805.71 + 420.30\ ln(B_1(H)) \quad (16)$$

$$FP = -640.27 + 168.152\ ln(B_1(H)) \quad (17)$$

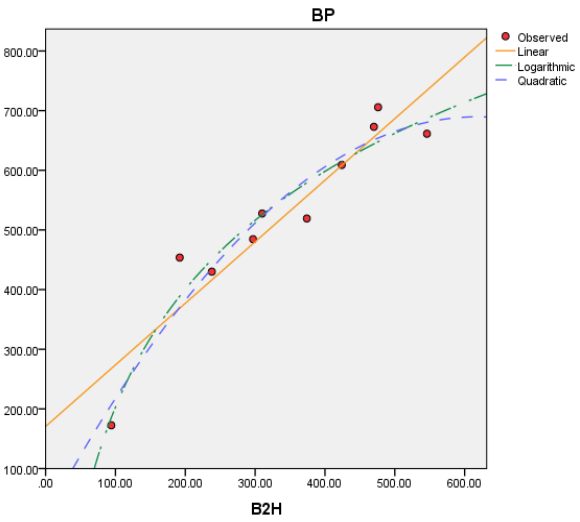


Figure 13a.Boiling point on B$_2$(H)

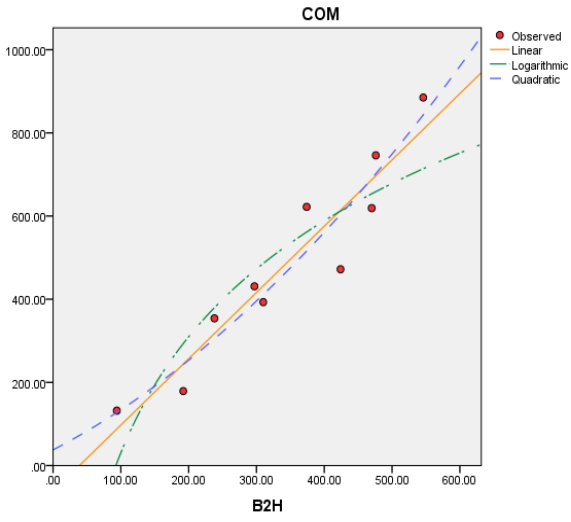


Figure 13b.Complexity on B$_2$(H)

https://doi.org/10.71058/jodac.v10i02006

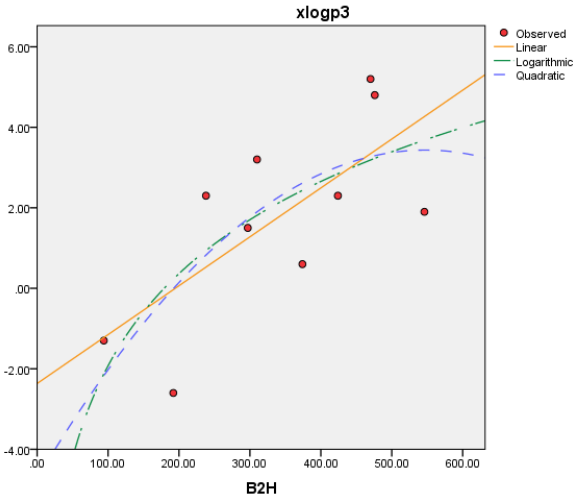


Figure 13c.XLogP$_3$ on B_2(H)

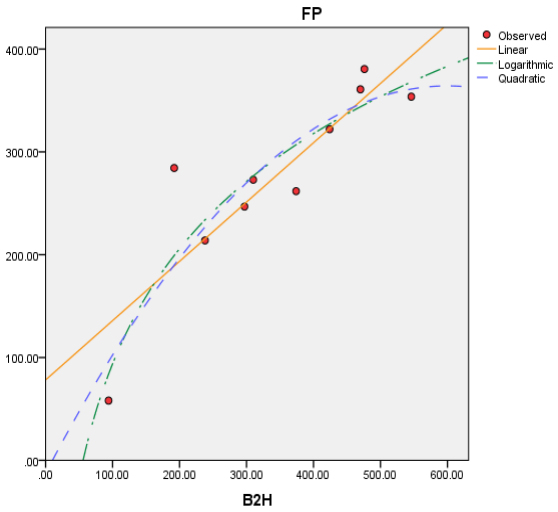


Figure 13d.Flash point on B_2(H)

Figure 13. Visual representations of the B_2(H) regression analysis.

The logarithmic regression model, which make use of HB_1(H),as follows for projecting the boiling point, complexity and flash point:

$$BP = -1537.15 + 288.56\ ln(HB_1(H)) \quad (18)$$

$$COM = -2423.38 + 407.02\ ln(HB_1(H)) \quad (19)$$

$$FP = -893.03 + 163.62\ ln(HB_1(H)) \quad (20)$$

The logarithmic regression models that employ B_2(H) to forecast boiling point, complexity, and flash point are listed below:

$$BP = -1110.02 + 285.11\ ln(B_2(H)) \quad (21)$$

$$COM = -1822.67 + 402.45\ ln(B_2(H)) \quad (22)$$

$$FP = -650.07 + 161.53\ ln(B_2(H)) \quad (23)$$

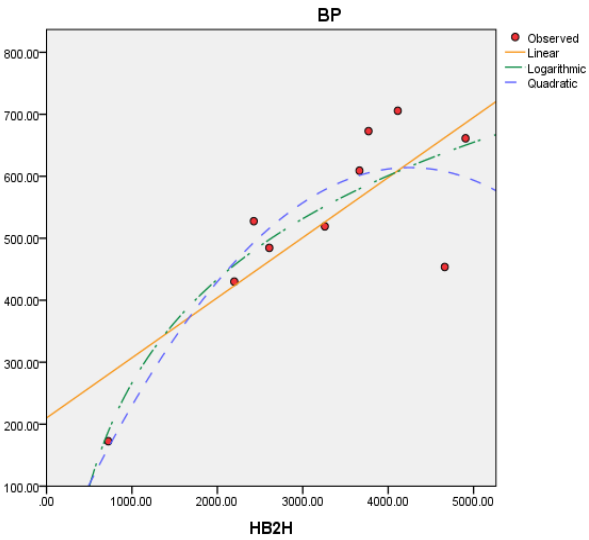


Figure 14a.Boiling point on HB_2(H)

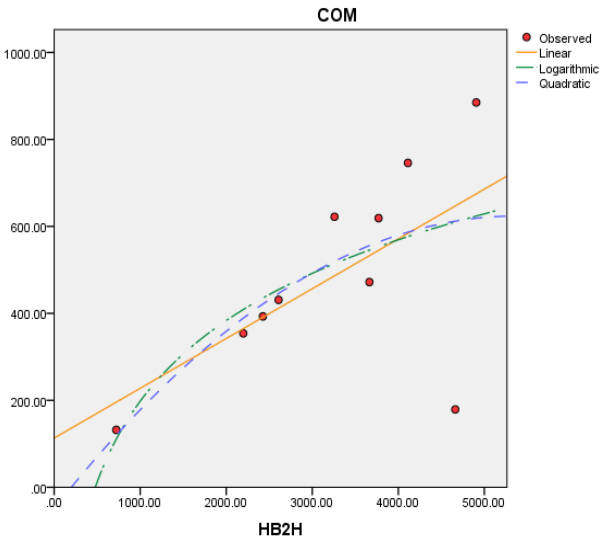


Figure 14b.Complexity on HB_2(H)

https://doi.org/10.71058/jodac.v10i02006

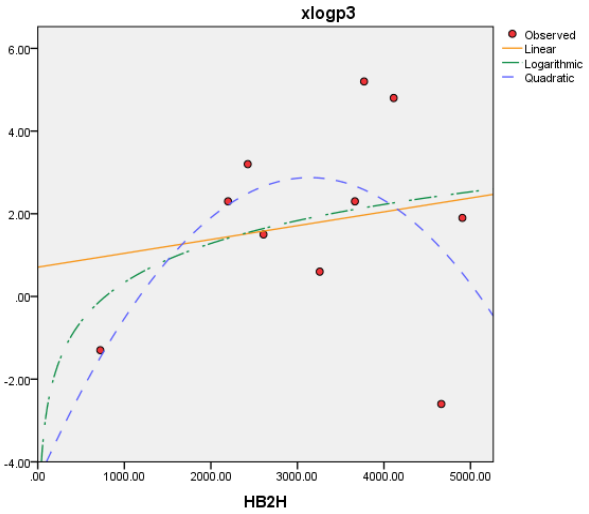


Figure 14c.XLogP$_3$ on HB$_2$(H)

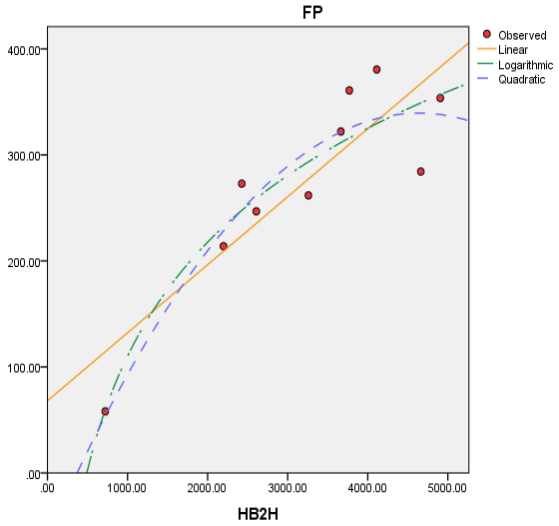


Figure 14d.Flash point on HB$_2$(H)

Figure 14. Visual representations of the HB$_2$(H) regression analysis.

The logarithmic regression models using HB$_2$(H) that are used to predict flash point are as follows:

$$FP = -961.41 + 155.12\ ln(HB_2(H)) \quad (24)$$

The logarithmic regression models using H$_b$(H) that are used to forecast boiling point are as follows:

$$BP = -480.23 + 335.72\ ln(H_b(H)) \quad (25)$$

Here is a listing of logarithmic regression models that employ BII$_1$(H) to anticipate boiling point and complexity:

$$BP = 152.51 + 4.662\ ln(BII_1(H)) \quad (26)$$

$$COM = -76.48 + 7.032\ ln(BII_1(H)) \quad (27)$$

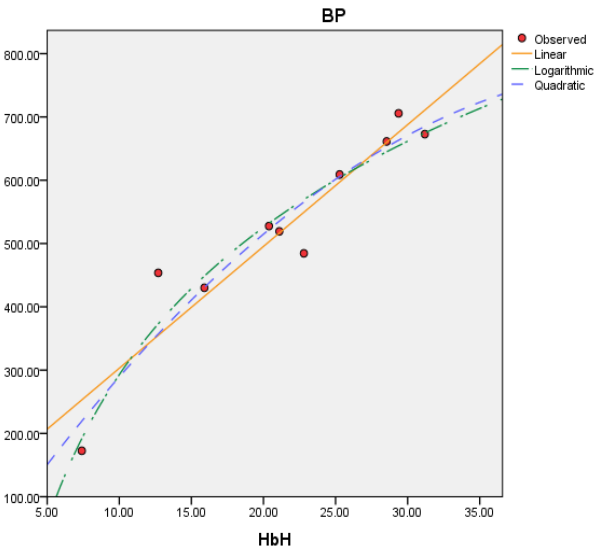


Figure 15a.Boiling point on H$_b$(H)

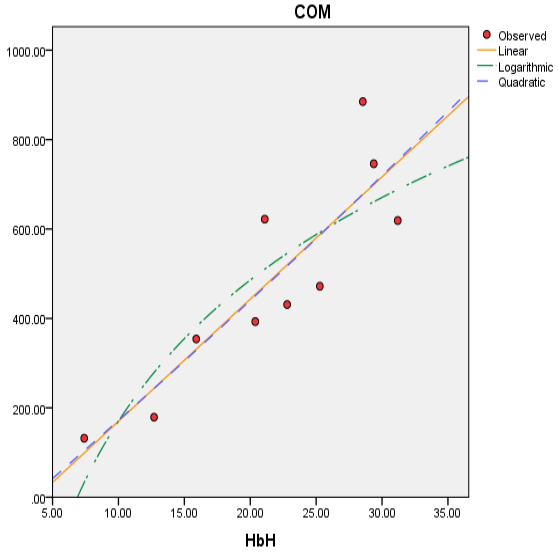


Figure 15b.Complexity on H$_b$(H)

https://doi.org/10.71058/jodac.v10i02006

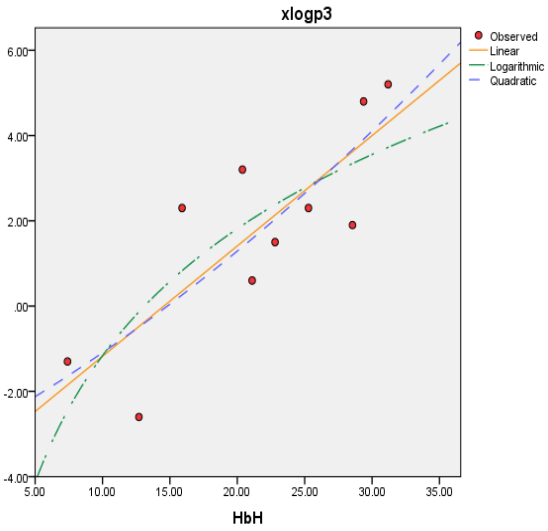


Figure 15c.XLogP$_3$ on H_b(H)

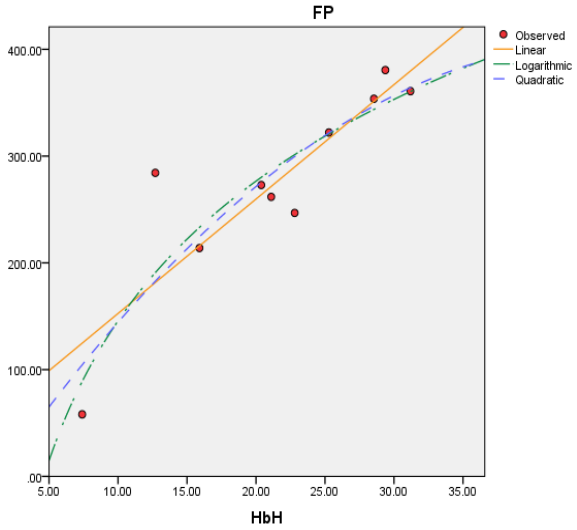


Figure 15d.Flash point on H_b(H)

Figure 15. Visual representations of the H_b(H) regression analysis.

The results of the logarithmic regression models, employing HBII1(H) for predicting boiling point and complexity, are as follows:

$$BP = 152.51 + 2.331\ ln(HBII_1(H)) \quad (28)$$

$$COM = -76.48 + 3.516\ ln(HBII_1(H)) \quad (29)$$

The logarithmic regression models uses BII_2(H) to estimate complexity and boiling point are as shows:

$$BP = 165.94 + 4.034\ ln(BII_2(H)) \quad (30)$$

$$COM = -63.89 + 6.172\ ln(BII_2(H)) \quad (31)$$

The following set of logarithmic regression models uses $HBII_2$(H) for predicting complexity and boiling point:

$$BP = 165.94 + 2.017\ ln(HBII_2(H)) \quad (32)$$

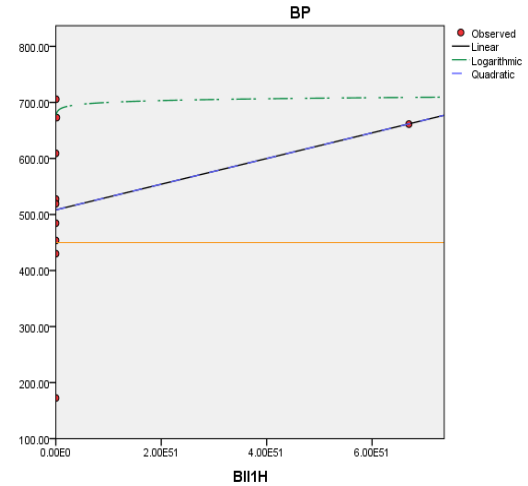


Figure 16a.Boiling point on BII_1(H)

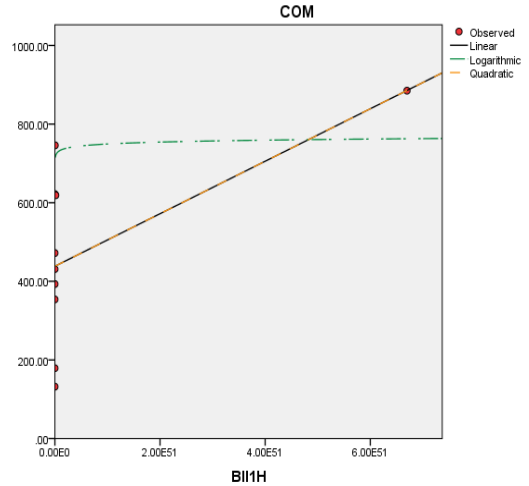


Figure 16b.Complexity on BII_1(H)

https://doi.org/10.71058/jodac.v10i02006

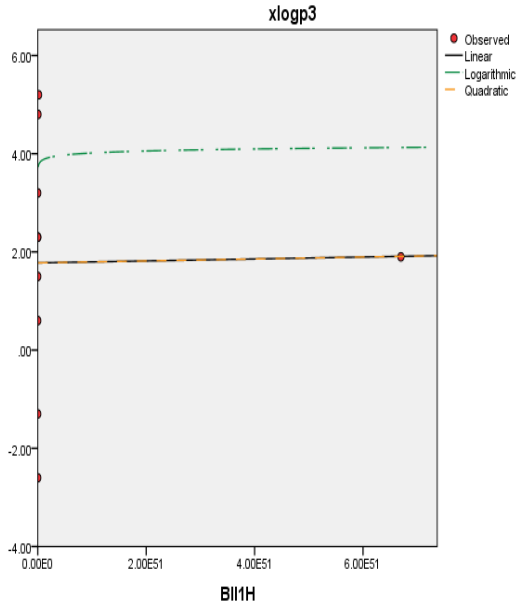


Figure 16c.XLogP$_3$ on BII$_1$(H)

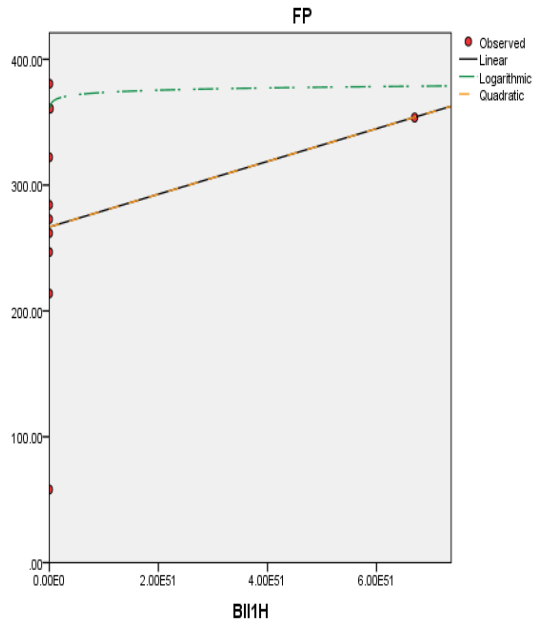


Figure 16d.Flash point on BII$_1$(H)

Figure 16. Visual representations of the BII$_1$(H) regression analysis.

$$COM = -63.89 + 3.086\ ln(HBII_2(H)) \quad (33)$$

The following presents the results of the logarithmic regression models, which use HII$_b$(H) for predicting complexity and boiling point:

$$BP = 162.96 - 8.0\ ln(HII_b(H)) \quad (34)$$

$$COM = -68.409 - 12.238\ ln(HII_b(H)) \quad (35)$$

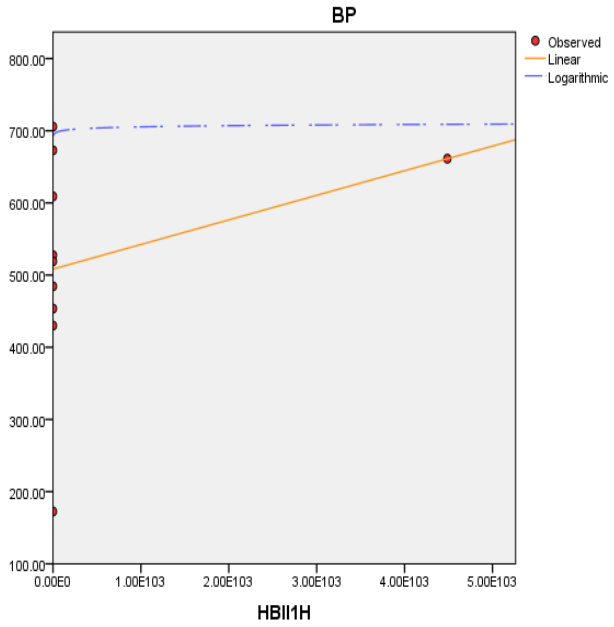


Figure 17a.Boiling point on HBII$_1$(H)

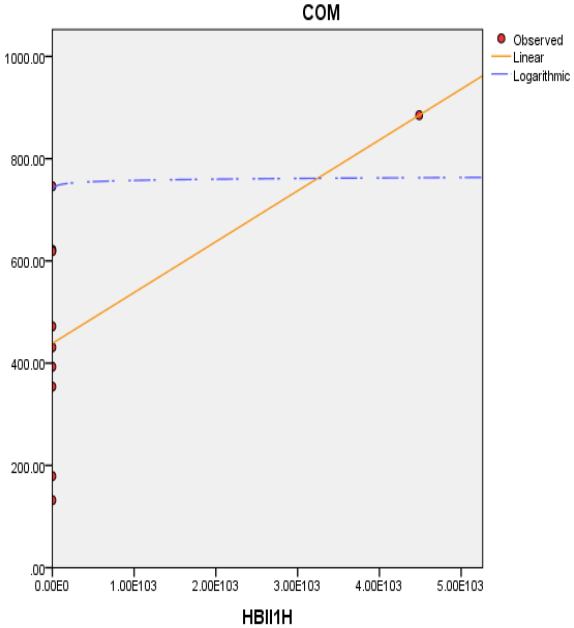


Figure 17b.Complexity on HBII$_1$(H)

https://doi.org/10.71058/jodac.v10i02006

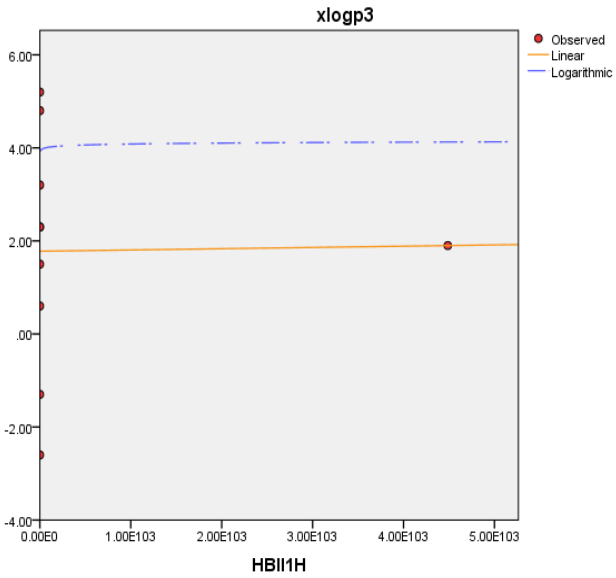


Figure 17c.XLogP$_3$ on HBII$_1$(H)

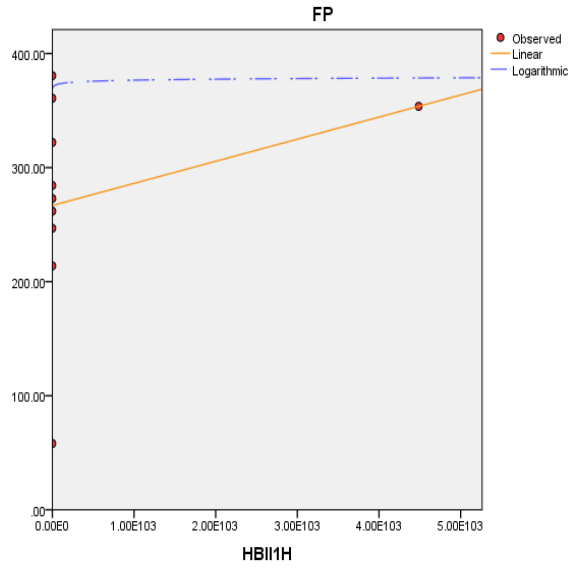


Figure 17d.Flash point on HBII$_1$(H)

Figure 17. Visual representations of the HBII$_1$(H) regression analysis.

The B$_1$(H) index regression model, which takes into account six physical features, is shown. A good tool for figuring out a medication's boiling point, complexity, and flash point is the B$_1$(H) index. (Fig.11)

The HB$_1$(H) index regression model, which takes into account six physical features, is displayed. The HB$_1$(H) index is a valid tool for determining the boiling point, complexity, and flash point of medications. (Fig.12)

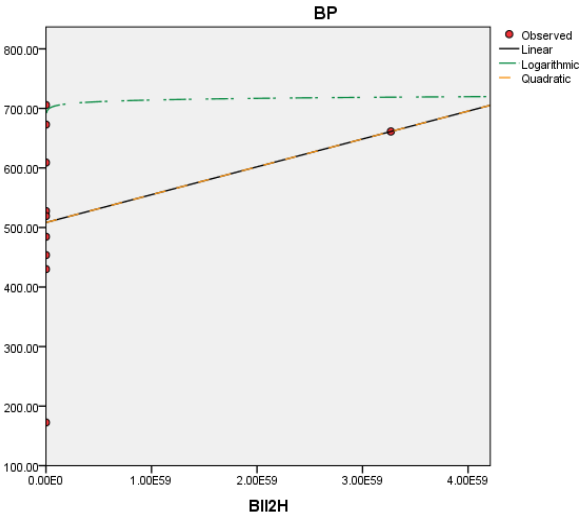


Figure 18a.Boiling point on BII$_2$(H)

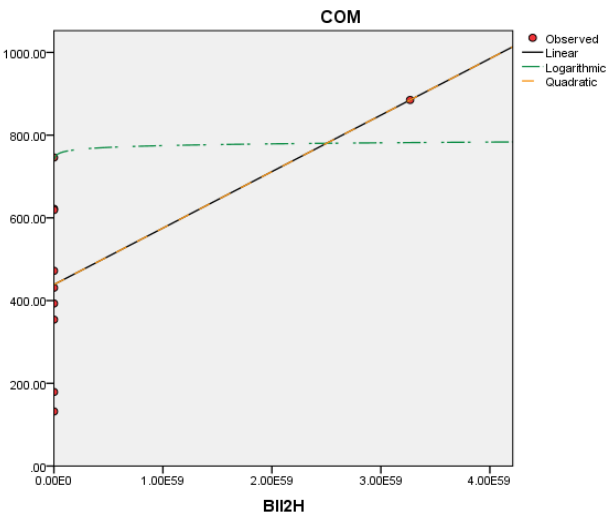


Figure 18b.Complexity on BII$_2$(H)

https://doi.org/10.71058/jodac.v10i02006

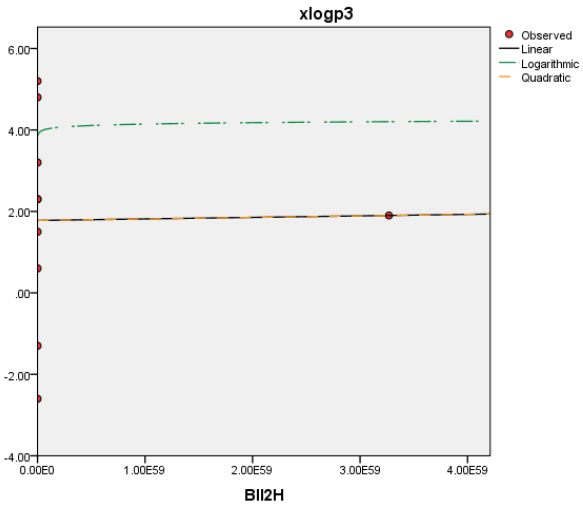


Figure 18c.XLogP_3 on $BII_2(H)$

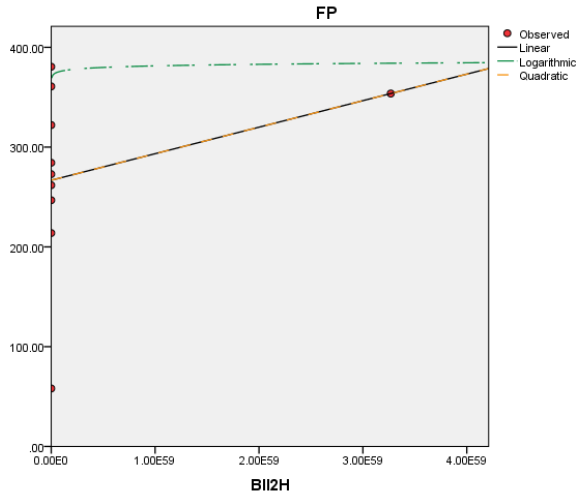


Figure 18d.Flash point on $BII_2(H)$

Figure 18. Visual representations of the $BII_2(H)$ regression analysis.

The $B_2(H)$ index regression model, which takes into account six physical features, is displayed. The $B_2(H)$ index is a proven tool for determining the boiling point, complexity, and flash point of medications. (Fig.13)

The $HB_2(H)$ index regression model, which takes into account six physical features, is displayed. One helpful technique for figuring out a medication's flash point is the $HB_2(H)$ index. (Fig.14)

The $H_b(H)$ index regression model, which takes into account six physical features, is displayed. One effective approach for figuring out a medication's boiling point is the $H_b(H)$ index. (Fig.15).

One of the physical attributes XlogP_3 cannot be predicted by these linear, quadratic and logarithmic regression models. The discussions that are made about the regression models of the multiplicative Banhatti indices are illustrated in the visual representations. (Fig. 16 to Fig.20) Based on the logarithmic regression models, the indices like $BII_1(H)$, $HBII_1(H)$, $BII_2(H)$, $HBII_2(H)$ and $HII_b(H)$ acts as a tool for predicting boiling point and complexity.

https://doi.org/10.71058/jodac.v10i02006

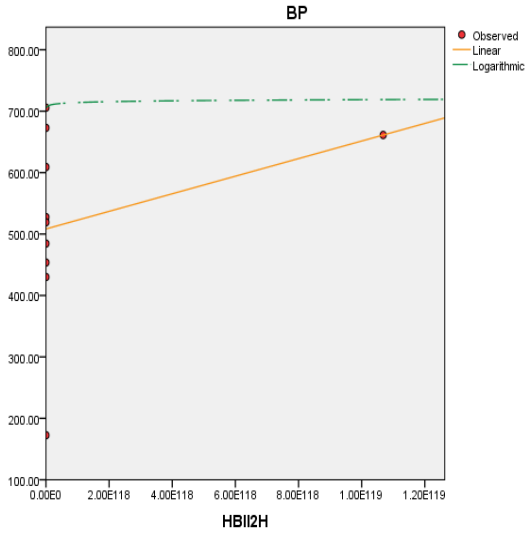


Figure 19a.Boiling point on $HBII_2(H)$

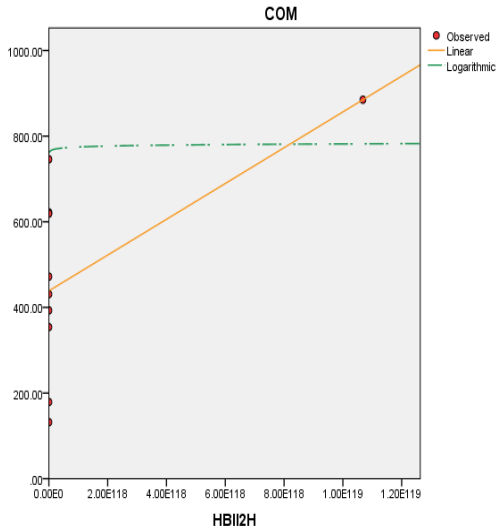


Figure 19b.Complexity on $HBII_2(H)$

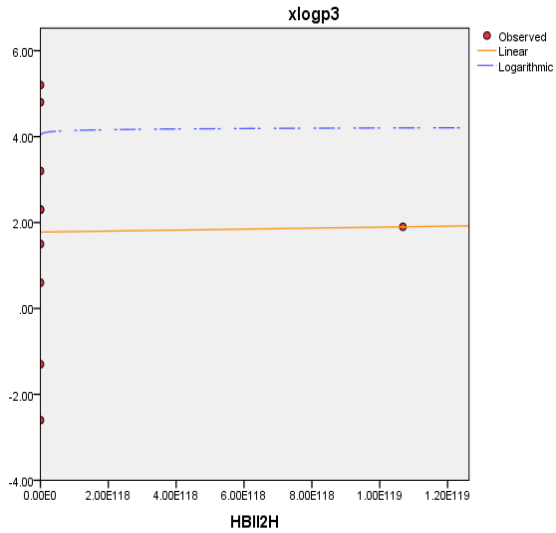


Figure 19c.$XLogP_3$ on $HBII_2(H)$

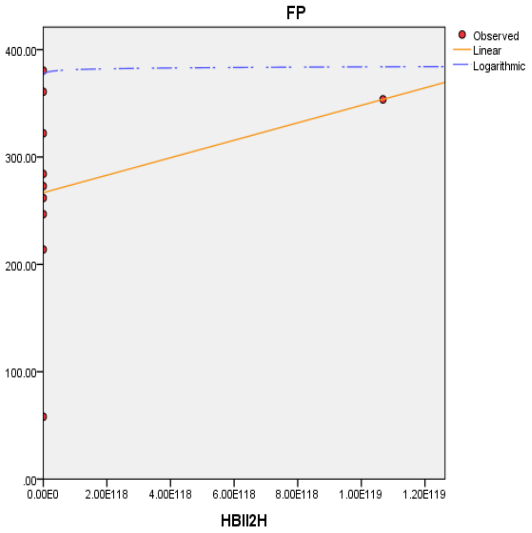


Figure 19d.Flash point on $HBII_2(H)$

Figure 19. Visual representations of the $HBII_2(H)$ regression analysis.

https://doi.org/10.71058/jodac.v10i02006

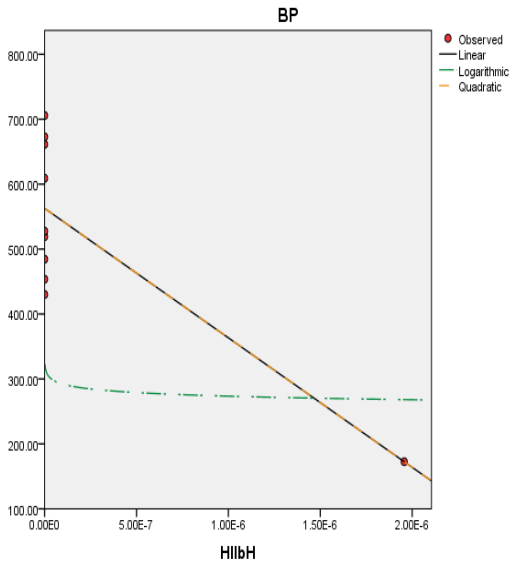


Figure 20a.Boiling point on $HII_b(H)$

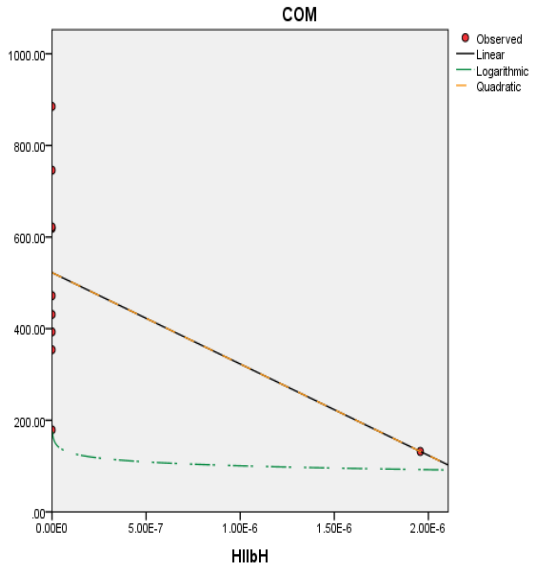


Figure 20b.Complexity on $HII_b(H)$

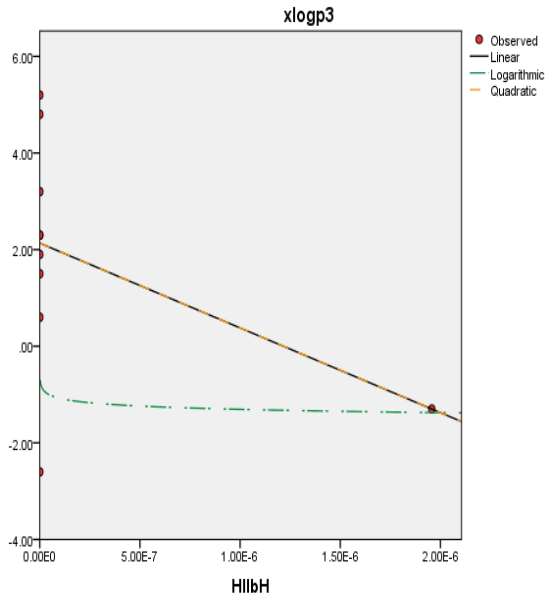


Figure 20c.XLogP$_3$ on $HII_b(H)$

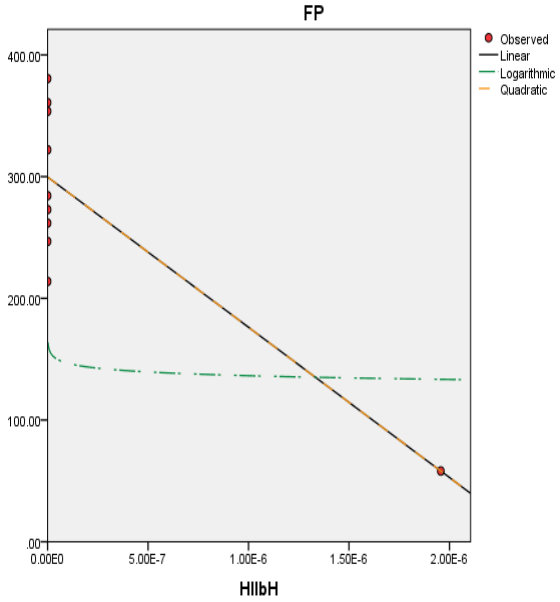


Figure 20d.Flash point on $HII_b(H)$

Figure 20. Visual representations of the $HII_b(H)$ regression analysis.

Conclusion

This study demonstrates the utility of Banhatti topological indices in analysing the molecular structures of diabetes related compounds such as Tolazamide, Dapagliflozin, Miglitol, Glibenclamide, Metformin, Alogliptin,Tolbutamide,Nateglinide,Repaglinide and Linagliptin. Regression models, including linear, quadratic, and logarithmic, reveal a significant relationship between the proposed indices and the physical and chemical parameters. The statistic indicates the amount of variance in the dependent variable that can be explained by the

https://doi.org/10.71058/jodac.v10i02006

independent variable. Considered the R value to be higher than 0.7 for the investigation. Based on the QSPR analysis, observe that in linear regression models,

- $B_1(H)$ and $H_b(H)$ index yields significant correlation coefficients for the parameters of boiling point.
- Complexity correlation is provided by the $HB_1(H)$ index.

In quadratic regression model,

- $HB_1(H)$ provides strong correlation coefficients for the parameters boiling point and complexity.
- $B_2(H)$ and complexity have a strong association.
- FP correlation is provided by $HB_2(H)$ index.

In logarithmic regression model,

- $B_1(H)$ and $HB_1(H)$ renders a profound correlation for the variables of boiling point.
- The multiplicative banhatti indices $BII_2(H)$, $HBII_2(H)$ and $HII_b(H)$ have a substantial correlation with complexity.
- FP and $HB_1(H)$ have a significant connection.

The application of these indices provided critical insights into the chemical and biological properties of molecules, involved in glucose regulation and insulin activity. These results suggest that Banhatti indices offer a reliable and efficient method for predicting the reactivity and stability of potential therapeutic agents for diabetes. The use of these indices may enhance the development of new treatments by offering a deeper understanding of molecular interactions relevant to diabetic pathways. Future studies should focus on expanding the scope of these indices to include a broader range of diabetic biomarkers and therapeutic molecules, potentially leading to breakthroughs in diabetes treatment strategies.

References

1. Parveen S, Hassan Awan NU, Mohammed M, Farooq FB, Iqbal N. Topological indices of novel drugs used in diabetes treatment and their QSPR modelling. Journal of Mathematics. 2022;2022(1):5209329. https://doi.org/10.1155/2022/5209329
2. Kumar A, Gangwar R, Ahmad Zargar A, Kumar R, Sharma A. Prevalence of diabetes in India: A review of IDF diabetes atlas 10th edition. Current diabetes reviews. 2024 Jan 1;20(1):105-14. https://doi.org/10.2174/1573399819666230413094200
3. Ibrahim RK, Ghudhaib KK, Allawi AA. Early Prediction of Nephropathy in Iraqi Patients with Diabetes Type II by Evaluating of some Relevant Biochemical Factors. Baghdad Sci J. 2023. https://dx.doi.org/10.21123/bsj.2023.8008
4. Leslie RD, Ma RC, Franks PW, Nadeau KJ, Pearson ER, Redondo MJ. Understanding diabetes heterogeneity: key steps towards precision medicine in diabetes. The Lancet Diabetes & Endocrinology. 2023 Nov 1;11(11):848-60.https://doi.org/10.1016/S2213-8587(23)00159-6
5. Hatem HM, Ghudhaib KK. Evaluation of Retinol Binding Protein 4 Level in Iraqi Patients with Type 2 Diabetes and Pre-diabetes Status as a Predictive Factor. Baghdad Science Journal. 2024.https://doi.org/10.21123/bsj.2024.9088

https://doi.org/10.71058/jodac.v10i02006

6. Tiwari P. Recent trends in therapeutic approaches for diabetes management: a comprehensive update. Journal of diabetes research. 2015;2015(1):340838. https://doi.org/10.1155/2015/340838
7. Van Netten JJ, Bus SA, Apelqvist J, Chen P, Chuter V, Fitridge R, Game F, Hinchliffe RJ, Lazzarini PA, Mills J, Monteiro-Soares M. Definitions and criteria for diabetes-related foot disease (IWGDF 2023 update). Diabetes/Metabolism Research and Reviews. 2024 Mar;40(3):e3654. https://doi.org/10.1002/dmrr.3654
8. Wagner S, Wang H. Introduction to chemical graph theory. Chapman and Hall/CRC; 2018 Sep 5. https://doi.org/10.1201/9780429450532
9. Trinajstic N. Chemical graph theory. CRC press; 2018 May11.https://doi.org/10.1201/9781315139111
10. Tang JH, Abid M, Ali K, Fahad A, Chaudhry MA, Qureshi MI, Liu JB. On Computation of Edge Degree-Based Banhatti Indices of a Certain Molecular Network. Journal of Mathematics. 2021;2021(1):5185270. https://doi.org/10.1155/2021/5185270
11. Mahboob A, Rasheed MW, Bayati JH, Hanif I. Computation of Several Banhatti and Reven Invariants of Silicon Carbides. Baghdad Science Journal. 2023 Jun 20;20(3 (Suppl.)):1099-. https://dx.doi.org/10.21123/bsj.2023.8212
12. Ravi V, Desikan K. Curvilinear regression analysis of benzenoid hydrocarbons and computation of some reduced reverse degree based topological indices for hyaluronic acid-paclitaxel conjugates. Scientific Reports. 2023 Feb 24;13(1):3239. https://doi.org/10.1038/s41598-023-28416-3
13. Alameri A, Yousef W. Topological and Hyper Topological Coindices of Benzenoid Circumcoronene Series. Baghdad Science Journal. 2024.https://doi.org/10.21123/bsj.2024.10588
14. Liu P, Long W. Current mathematical methods used in QSAR/QSPR studies. International Journal of Molecular Sciences. 2009 Apr 29;10(5):1978-98. https://doi.org/10.3390/ijms10051978
15. Mekala A, Murali R. Some K-Banhatti Polynomials of First Dominating David Derived Networks. Baghdad Science Journal. 2023 Apr 1;20(2):0349-. http://dx.doi.org/10.21123/bsj.2022.6996
16. Kulli VR. K Banhatti indices of chloroquine and hydroxychloroquine: Research Applied for the treatment and prevention of COVID-19. SSRG International Journal of Applied Chemistry. 2020;7(1):63-8. https://www.internationaljournalssrg.org/IJAC/2020/Volume7-Issue1/IJAC-V7I1P113.pdf
17. Kulli VR. On K Banhatti indices of graphs. Journal of Computer and Mathematical Sciences. 2016 Apr;7(4):213-8. http://www.compmath-journal.org/
18. Kulli VR, On K. On K hyper-Banhatti indices and coindices of graphs. International Research Journal of Pure Algebra. 2016;6(5):300-https://www.researchgate.net/publication/302563493_On_K_hyper-Banhatti_indices_and_coindices_of_graphs
19. Wang W, Naeem M, Rauf A, Riasat A, Aslam A, Anoh Yannick K. [Retracted] On Analysis of Banhatti Indices for Hyaluronic Acid Curcumin and Hydroxychloroquine. Journal of Chemistry. 2021;2021(1):7468857. https://doi.org/10.1155/2021/7468857

https://doi.org/10.71058/jodac.v10i02006

20. Farooq FB, Parveen S, Hassan Awan NU, Fanja R. Topological Descriptors and QSPR Modelling of HIV/AIDS Disease Treatment Drugs. Discrete Dynamics in Nature and Society. 2023;2023(1):9963241. https://doi.org/10.1155/2023/9963241
21. Yasin HM, Suresh M, Tefera ZG, Fufa SA. M-Polynomial and NM-Polynomial Methods for Topological Indices of Polymers. Int J Math Math Sci. 2024; 2024(1): 1-16. Available from: https://onlinelibrary.wiley.com/doi/epdf/10.1155/2024/1084450. DOI: https://doi.org/10.1155/2024/1084450
22. Parveen S, Awan NU, Farooq FB, Fanja R, Anjum QU. Topological indices of novel drugs used in autoimmune disease vitiligo treatment and its QSPR modeling. BioMed Research International. 2022;2022(1):6045066. https://doi.org/10.1155/2022/6045066
23. Huang R, Mahboob A, Rasheed MW, Alam SM, Siddiqui MK. On molecular modeling and QSPR analysis of lyme disease medicines via topological indices. The European Physical Journal Plus. 2023 Mar 15;138(3):243. https://doi.org/10.1140/epjp/s13360-023-03867-9
24. Hosamani S, Perigidad D, Jamagoud S, Maled Y, Gavade S. QSPR analysis of certain degree based topological indices. Journal of Statistics Applications & Probability. 2017;6(2):361-71. http://dx.doi.org/10.18576/jsap/060211
25. Bokhary SA, Adnan, Siddiqui MK, Cancan M. On topological indices and QSPR analysis of drugs used for the treatment of breast cancer. Polycyclic Aromatic Compounds. 2022 Oct 21;42(9):6233-53.https://doi.org/10.1080/10406638.2021.1977353
26. Zhang X, Reddy HG, Usha A, Shanmukha MC, Farahani MR, Alaeiyan M. A study on anti-malaria drugs using degree-based topological indices through QSPR analysis. Math. Biosci. Eng. 2023 Jan 1;20(2):3594-609. http://doi.org/10.3934/mbe.2023167
27. Gnanaraj LR, Ganesan D, Siddiqui MK. Topological indices and QSPR analysis of NSAID drugs. Polycyclic Aromatic Compounds. 2023 Nov 26;43(10):9479-95.https://doi.org/10.1080/10406638.2022.2164315
28. Yasin H, Mohammed; M, Suresh; and Bayati, Jalal Hatem Hussein (2025) "Topological Indices and QSPR/QSAR Analysis of Some Drugs Being Investigated for the Treatment of Alzheimer's Disease Patients," *Baghdad Science Journal*: Vol. 22: Iss. 1, Article 23. DOI: https://doi.org/10.21123/bsj.2024.10866