European Journal of Molecular & Clinical Medicine
ISSN 2515-8260 Volume 07, Issue 10, 2020

Degree-Based Topological Indices on Asthma Drugs with QSPR Analysis during Covid-19

Anil Kumar K N[1], Basavarajappa N S[2], Shanmukha M C [3], Shilpa K C[4]
[1,2]Department of Mathematics
[4]Department of Computer Science & Engg.
Bapuji Institute of Engineering and Technology, Davanagere-577004
and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka, India
[3]Department of Mathematics,
Jain Institute of Technology, Davanagere-577003
and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka, India
E-mail: [1*]kn.anil5340@gmail.com, [2]dr.nsbasavaraj@gmail.com,
[3]mcshanmukha@gmail.com,[4]shilpastjit21@gmail.com

***Abstract**: Asthma is a condition where a person's airways became inflamed, narrow and swell and produce extra mucus which makes the person difficult to breath. There are some drugs used as a controller medicine for asthma. In this work, topological indices are used to determine the physical and chemical characteristics of asthma drugs. In the pandemic situation most of the people are dying from Covid-19 who were suffering from BP, Diabetes and Respiratory related (asthma) problems. This may help the chemists to understand the characteristics of drugs used in the treatment of asthma along with Covid-19.*

Keywords: Topological indices, Asthma drugs, Pharmaceutical chemistry, QSPR Analysis.

1. INTRODUCTION AND TERMINOLOGIES

The framework used to apply the concepts of mathematics to chemistry in research area is mathematical chemistry. It includes the mathematical modelling of chemical mechanism. The existing area of mathematics having various applications in chemistry is graph theory called chemical graph theory.

Asthma is one of the most common non-communicable disease. Globally, it affects 1−18% of the population according to the Global Initiative for Asthma (*GINA*). Asthma is defined as a heterogeneous disease, which is mainly characterized by chronic inflammation of the airways, particularly lower airways. It is also associated with hyper responsiveness of tracheobronchial smooth muscle to a variety of Stimuli, which leads to narrowing of air tubes, accompanied by mucus plugging. Common symptoms of asthma includes cough, chest tightness, wheezing and shortness of breath. Chemical mediators responsible for asthma includes histamine, protease enzymes, TNF_{α} , Prostaglandins (PG_s), Leukotrienes (LT_s), Interleukins (IL_s). All these are produced by mast cells (present in lungs) and inflammatory cells. These mediators together constrict bronchial smooth muscle, cause mucosal oedema, hyperemia and produce viscid secretions, all results in reversible airway obstruction.

The treatment of asthma includes antagonising the released mediators and bronchodilators. The mediator inhibiting drugs *Montelukast, Pranlukast, Zafirlukast* acts by competitively antagonizing the $CysLT_1$ (Cystenyl Leukotrienes) receptor mediated bronchoconstriction, increased vascular permeability and recruitment of eosinophils. Thereby relieving the symptoms of asthma. The DP_2 receptor antagonist drugs *Ramatroban, Setipiprant, Fevipiprant* acts by antagonising the action of DP_2 receptor and thereby blocking bronchoconstriction, hyperresponsiveness of the airways and infiltration of inflammatory cells. The antihistamine drug *Toreforant* inhibits the action of histamine responsible for brochoconstriction which relieves the symptoms of asthma. The Bronchodilators *Salbutamol, Terbutaline, Salmeterol* drugs causes Bronchodilatation through β_2 receptor stimulation. These increases *cAMP* formation in bronchial muscle cell which leads to bronchial muscle relaxation [15].

Nowadays, the Covid-19 pandemic is an uncontrollable disease which is not having any drug to cure it. The people are suffering from asthma have chance of suffering from Covid-19. Out of childhood asthma and adult-onset asthma, there is a report evident that adult-onset asthma may increase the risk of hospitalization from Covid-19 above 50 years of age group. Earlier information says that steroids were not suitable in patients with Covid-19 disease, even though there is a usefulness of steroids in Covid-19 disease. After many discussions on the use of steroids, the solution is continue taking controller medicine and do not stop them. In the current pandemic, the best thing a person suffering from asthma is to keep their asthma under the control.

QSAR/QSPR are the important tools in chemical and medical fields, helps to analyse the physical and chemical characteristics with biological activities. First, the correlation between chemical compound and physico-chemical characteristic or biological activity is determined. Then, physico-chemical characteristic or biological activity of structurally related compounds are predicted [2, 8, 10, 11, 12, 13, 18 and 19].

In theoretical chemistry, chemical compound is depicted as molecular graph with vertices and edges. The vertex set is denoted as atoms and edge set as links between the atoms. Consider *G* (*V, E*) be a molecular graph with vertices and edges respectively. The degree of a vertex in *G* is $\xi(s)$ of vertex (atom) *s*. The simple, finite and loop free graphs are used in this study [1, 6, 14].

2. DEGREE-BASED TOPOLOGICAL INDICES OF GRAPH

Definition 2.1. *Gutman et al. [7] proposed the first and second Zagreb indices as*

$$M_1(G) = \sum_{e=st \in E(G)} (\xi(s) + \xi(t)) .$$

$$M_2(G) = \sum_{e=st\in E(G)} (\xi(s) \times \xi(t)) .$$

Definition 2.2. *Harmonic index is proposed by Fajtlowicz [4] as,*

$$H(G) = \sum_{e=st\in E(G)} \frac{2}{\xi(s) + \xi(t)} .$$

Definition 2.3. *G.H. Shirdel et al. [14] introduced the Hyper Zagreb index as*

$$HM(G) = \sum_{e=st\in E(G)} [\xi(s) + \xi(t]^2 .$$

Definition 2.4. *B. Furtula et al. [6] introduced the forgotten topological index as*

$$F(G) = \sum_{e=st\in E(G)} [\xi(s)]^2 + [\xi(t)]^2 .$$

Definition 2.5. *Milan Randic defined Randic index [9] as*

$$R(G) = \sum_{e=st\in E(G)} \frac{1}{\sqrt{\xi(s)\,\xi(t)}} .$$

Definition 2.6. *O. Favaron et al. [5] defined Reciprocal Randic index as,*

$$RR(G) = \sum_{e=st\in E(G)} \sqrt{\xi(s) \times \xi(t)} .$$

Definition 2.7. *Zhou et al. [17] introduced the sum-connectivity index as*

$$SCI(G) = \sum_{e=st\in E(G)} \frac{1}{\sqrt{\xi(s) + \xi(t)}} .$$

.

Definition 2.8. *Vukicevic et al. [16] proposed the Geometric arithmetic index as*

$$GA(G) = \sum_{e=st\in E(G)} \frac{2\sqrt{\xi(s) \times \xi(t)}}{\xi(s) + \xi(t)} .$$

.

Definition 2.9. *Estrada et al. [3] proposed Atom bond connectivity index as*

$$ABC(G) = \sum_{e=st \in E(G)} \sqrt{\frac{\xi(s) + \xi(t) - 2}{\xi(s) \times \xi(t)}} .$$

3. MATERIALS AND METHODS

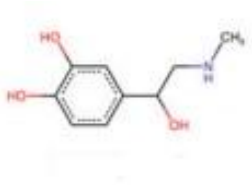
The materials used for this work are the Asthma Drug molecules choosen from [15]. For computation of results, the tools employed are graph theoretical tools, analytic techniques and degree counting methods based on vertices and edges of chemical structures.

In order to find the topological indices of 19 asthma drug molecules, each molecule is considered as a graph. The links between the atoms are considered as edges and the atoms of each links are considered as vertices of that molecule. The degree of every vertex and the types of edges are studied for each molecule. Topological index is a numerical measure, which follows a specific rule.

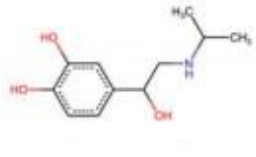
DEGREE-BASED TOPOLOGICAL INDICES IN QSPR STUDIES

In this proposed work, 10 degree-based topological indices are discussed viz.1^{st}-Zagreb, 2^{nd}-Zagreb, Harmonic, Hyper Zagreb, Forgotten, Randic, Reciprocal Randic, Sum-Connectivity, Geometric Arithmetic and ABC indices for modelling five physical and chemical characteristics [Boiling point(BP), Enthalpy(E), Flash point(FP), logP, Molar Volume(MV)] of nineteen asthma drug molecules from *Epinephrine* to *Toreforant*. Using Chem-spider the values of above physico-chemical properties are taken.

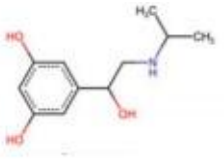
The above calculated values of defined degree-based topological indices and the experimental values of physical and chemical characteristics of nineteen asthma drugs (Figure 1) are represented respectively from Table 1 to 3.



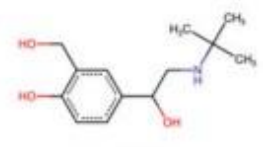
(a) Epinephrine



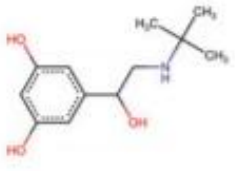
(b) Isoproterenol



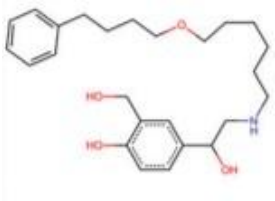
(c) Metaproterenol



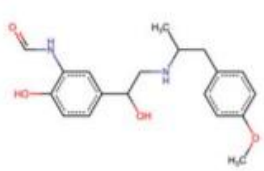
(d) Salbutamol



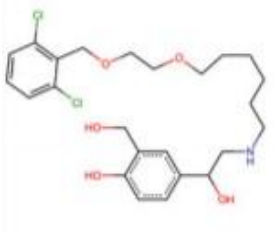
(e) Terbutaline



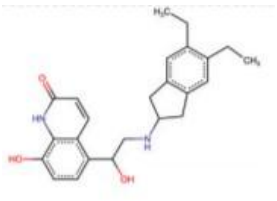
(f) Salmeterol



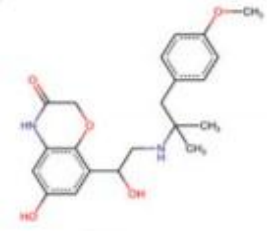
(g) Formoterol



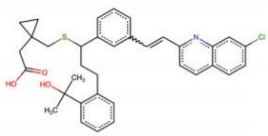
(h) Olodaterol



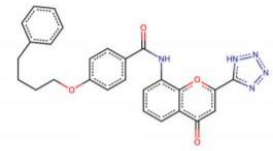
(i) Indacaterol



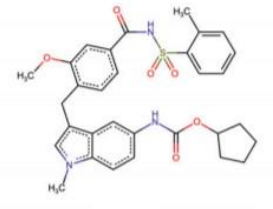
(j) Vilanterol



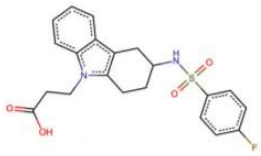
(k) Montelukast



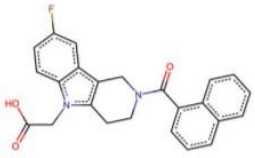
(l) Pranlukast



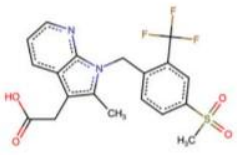
(m) Zafirlukast



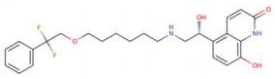
(n) Ramatroban



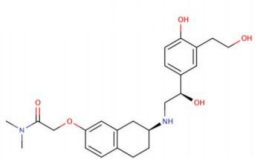
(o) Setipiprant



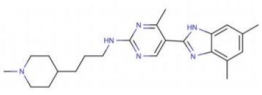
(p) Fevipiprant



(q) Abediterol



(r) Bedoradrine



(s) Toreforant

Figure 1: Molecular structures of various Asthma drugs.

Table 1: Various drug molecules of Asthma with Physico-chemical properties

Molecules	***BP***	***E***	***FP***	***logP***	***MV***
Epinephrine	413.1	70.2	207.9	−0.63	142.7
Isoproterenol	417.5	70.7	179.7	0.25	176.1
Metaproterenol	417.5	70.7	179.7	0.13	176.1
Salbutamol	433.5	72.7	159.5	0.01	207.6
Terbutaline	419.2	70.9	165.3	0.48	192.3
Salmeterol	603	94.3	318.5	3.07	373.7
Formoterol	603.2	94.3	318.6	1.57	279.1
Olodaterol	649	100.5	346.3	1.17	308.9
Indacaterol	660.3	102.1	353.1	3.88	306.9
Vilanterol	646.7	100.2	344.9	2.97	387.5
Montelukast	750.5	114.8	407.7	7.8	460.8
Pranlukast	–	–	–	3.88	350.4
Zafirlukast	–	–	–	6.15	433.6
Ramatroban	654.7	101.3	349.7	4.09	289.7
Setipiprant	690.4	106.3	371.4	3.39	292.4
Fevipiprant	637.6	99	339.4	2.85	295.4
Abediterol	681.6	105	366	3.67	371.3
Bedoradrine	695.9	107	374.7	0.12	335.4
Toreforant	611.2	90.8	323.4	4.22	341.7

Table 2: Various drug molecules of Asthma with Topological Indices Values

Molecules	$M_1(G)$	$M_2(G)$	$H(G)$	$HM(G)$	$F(G)$	$R(G)$
Epinephrine	60	67	5.833	286	152	6.147
Isoproterenol	70	77	6.566	334	180	7.003
Metaproterenol	70	76	6.533	332	180	6.986
Salbutamol	82	90	7.266	406	226	7.832
Terbutaline	78	84	6.666	386	218	7.277
Salmeterol	136	148	14.433	610	314	14.703
Formoterol	120	135	11.6	568	298	12.028
Olodaterol	146	168	12.633	726	390	13.270
Indacaterol	156	187	13.533	780	406	13.995
Vilanterol	148	164	15.1	682	354	15.524
Montelukast	220	256	18.819	1100	588	19.60
Pranlukast	188	219	17.366	902	464	17.67
Zafirlukast	220	260	18.886	1102	582	19.64
Ramatroban	157	185	13.386	791	421	14.017

Setipiprant	168	205	14.1	850	440	14.525
Fevipiprant	158	187	12.471	826	452	13.392
Abediterol	164	187	15.352	792	418	15.882
Bedoradrine	156	179	14.3	754	396	14.867
Toreforant	154	180	13.53	754	394	13.991

Table 3: Various drug molecules of Asthma with Topological Indices Values

Molecules	***RR*(*G*)**	***SCI*(*G*)**	***GA*(*G*)**	***ABC*(*G*)**
Epinephrine	28.858	6.130	12.44	9.44
Isoproterenol	33.357	6.999	14.209	11.073
Metaproterenol	33.256	6.986	14.168	11.113
Salbutamol	38.404	7.827	15.896	12.635
Terbutaline	36.171	7.289	14.799	12.078
Salmeterol	66.924	14.919	30.493	22.058
Formoterol	58.317	12.232	25.201	18.632
Olodaterol	70.01	13.721	28.723	21.738
Indacaterol	76.115	14.654	31.12	22.713
Vilanterol	72.388	15.735	32.225	23.61
Montelukast	105.964	20.522	43.355	32.442
Pranlukast	92.555	18.591	39.368	28.3
Zafirlukast	106.524	20.546	43.495	32.271
Ramatroban	75.615	14.588	30.754	23.12
Setipiprant	82.221	15.435	33.181	24.115
Fevipiprant	74.619	13.861	35.175	22.836
Abediterol	79.534	16.338	33.949	25.171
Bedoradrine	75.716	15.313	31.93	23.72
Toreforant	75.019	14.683	31.1	22.902

4. REGRESSION MODELS

From the above tables 1 to 3, it is observed that values are normally distributed. Hence regression analysis is used for computation. Now, linear regression model is checked as follows.

$$P = A + B\,(TI) \qquad (1)$$

such that P represents physical property, TI is the topological index and A and B are constants. These values are computed through *SPSS* software to analyse the values of five physical and chemical characteristics and the ten topological indices of nineteen asthma

drugs. Using equation 1, several linear models are obtained for the defined degree-based topological indices. They are as follows,

4.1 First Zagreb index $M_1(G)$:

$BP = 252.255 + 2.54[M_1(G)]$
$E = 49.075 + 0.328[M_1(G)]$
$FP = 64.286 + 1.789[M_1(G)]$
$logP = -3.215 + 0.042[M_1(G)]$
$MV = 62.511 + 1.710[M_1(G)]$

4.2 Second Zagreb index $M_2(G)$:

$BP = 274.032 + 2.068[M_2(G)]$
$E = 51.905 + 0.267[M_2(G)]$
$FP = 79.305 + 1.459[M_2(G)]$
$logP = -2.862 + 0.034[M_2(G)]$
$MV = 83.018 + 1.357[M_2(G)]$

4.3 Harmonic index $H(G)$:

$BP = 240.04 + 29.211[H(G)]$
$E = 47.52 + 3.775[H(G)]$
$FP = 53.456 + 20.765[H(G)]$
$logP = -3.288 + 0.0468[H(G)]$
$MV = 40.058 + 20.81[H(G)]$

a. **Hyper Zagreb index $HM(G)$:**

$BP = 270.783 + 0.49[HM(G)]$
$E = 51.432 + 0.63[HM(G)]$
$FP = 78.106 + 0.344[HM(G)]$
$logP = -2.991 + 0.008[HM(G)]$
$MV = 79.677 + 0.324[HM(G)]$

b. **Forgotten topological index $F(G)$:**

$BP = 270.522 + 0.924[F(G)]$
$E = 51.348 + 0.12[F(G)]$
$FP = 78.953 + 0.646[F(G)]$
$logP = -3.069 + 0.016[F(G)]$
$MV = 78.287 + 0.616[F(G)]$

c. **Randic index $R(G)$:**

$BP = 227.83 + 28.961[R(G)]$
$E = 45.909 + 3.745[R(G)]$
$FP = 45.431 + 20.534[R(G)]$
$logP = -3.508 + 0.466[R(G)]$
$MV = 31.533 + 20.626[R(G)]$

d. **Reciprocal Randic index $RR(G)$:**

$BP = 256.49 + 5.196[RR(G)]$
$E = 49.652 + 0.671[RR(G)]$
$FP = 66.674 + 3.67[RR(G)]$
$logP = -3.109 + 0.084[RR(G)]$
$MV = 65.818 + 3.489[RR(G)]$

e. **Sum-connectivity index $SCI(G)$:**

$BP = 239.259 + 27.24[SCI(G)]$
$E = 47.421 + 3.52[SCI(G)]$
$FP = 53.527 + 19.315[SCI(G)]$
$logP = -3.327 + 0.438[SCI(G)]$
$MV = 43.625 + 19.085[SCI(G)]$

f. **Geometric Arithmetic index $GA(G)$:**

$BP = 254.85 + 12.322[GA(G)]$
$E = 49.46 + 1.592[GA(G)]$
$FP = 64.169 + 8.753[GA(G)]$
$logP = -3.107 + 0.2[GA(G)]$
$MV = 58.668 + 8.506[GA(G)]$

5.10. Atom Bond Connectivity index $ABC(G)$:

$BP = 233.037 + 17.747[ABC(G)]$
$E = 46.588 + 2.295[ABC(G)]$
$FP = 50.338 + 12.522[ABC(G)]$
$logP = -3.495 + 0.29[ABC(G)]$
$MV = 41.905 + 12.315[ABC(G)]$

Table 4: Statistical framework for the linear QSPR model for $M_1(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	252.255	2.54	**0.97**	0.0001	*significant*
Enthalpy	17	49.075	0.328	0.963	0.0001	*significant*
FlashPoint	17	64.286	1.789	0.945	0.0001	*significant*
logP	19	−3.215	0.042	0.882	0.0001	*significant*
Molar Volume	19	62.511	1.710	0.921	0.0001	*significant*

Table 5: Statistical framework for the linear QSPR model for $M_2(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	274.032	2.068	**0.966**	0.0001	*significant*
Enthalpy	17	51.905	0.267	0.959	0.0001	*significant*

FlashPoint	17	79.305	1.459	0.943	0.0001	*significant*
logP	19	−2.862	0.034	0.879	0.0001	*significant*
Molar Volume	19	83.018	1.357	0.894	0.0001	*significant*

Table 6: Statistical framework for the linear QSPR model for $H(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	240.04	29.211	0.964	0.0001	*significant*
Enthalpy	17	47.52	3.775	0.957	0.0001	*significant*
FlashPoint	17	53.456	20.765	0.949	0.0001	*significant*
logP	19	−3.288	0.0468	0.855	0.0001	*significant*
Molar Volume	19	40.058	20.81	**0.965**	0.0001	*significant*

Table 7: Statistical framework for the linear QSPR model for $HM(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	270.783	0.49	**0.954**	0.0001	*significant*
Enthalpy	17	51.432	0.63	0.949	0.0001	*significant*
FlashPoint	17	78.106	0.344	0.928	0.0001	*significant*
logP	19	−2.991	0.008	0.880	0.0001	*significant*
Molar Volume	19	79.677	0.324	0.887	0.0001	*significant*

Table 8: Statistical framework for the linear QSPR model for $F(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	270.522	0.924	**0.941**	0.0001	*significant*
Enthalpy	17	51.348	0.12	0.936	0.0001	*significant*
FlashPoint	17	78.953	0.646	0.909	0.0001	*significant*
logP	19	−3.069	0.016	0.877	0.0001	*significant*
Molar Volume	19	78.287	0.616	0.877	0.0001	*significant*

Table 9: Statistical framework for the linear QSPR model for $R(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	227.83	28.961	**0.967**	0.0001	*significant*
Enthalpy	17	45.909	3.745	0.961	0.0001	*significant*
FlashPoint	17	45.431	20.534	0.949	0.0001	*significant*
logP	19	−3.508	0.466	0.861	0.0001	*significant*

Molar Volume	19	31.533	20.626	0.966	0.0001	*significant*

Table 10: Statistical framework for the linear QSPR model for $RR(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	256.49	5.196	**0.974**	0.0001	*significant*
Enthalpy	17	49.652	0.671	0.967	0.0001	*significant*
FlashPoint	17	66.674	3.67	0.952	0.0001	*significant*
logP	19	−3.109	0.084	0.881	0.0001	*significant*
Molar Volume	19	65.818	3.489	0.924	0.0001	*significant*

Table 11: Statistical framework for the linear QSPR model for $SCI(G)$

Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	239.259	27.24	**0.971**	0.0001	*significant*
Enthalpy	17	47.421	3.52	0.964	0.0001	*significant*
FlashPoint	17	53.527	19.315	0.953	0.0001	*significant*
logP	19	−3.327	0.438	0.867	0.0001	*significant*
Molar Volume	19	43.625	19.085	0.958	0.0001	*significant*

Table 12: Statistical framework for the linear QSPR model for $GA(G)$

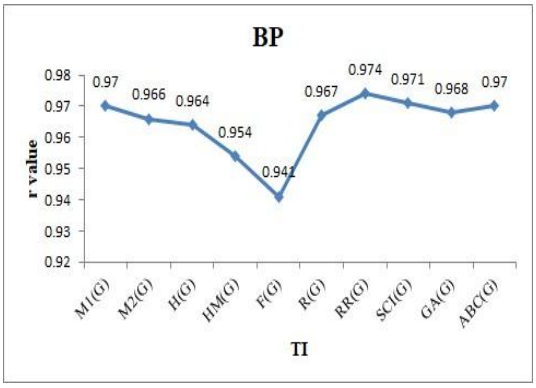
Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	254.85	12.322	**0.968**	0.0001	*significant*
Enthalpy	17	49.46	1.592	0.961	0.0001	*significant*
FlashPoint	17	64.169	8.753	0.952	0.0001	*significant*
logP	19	−3.107	0.2	0.864	0.0001	*significant*
Molar Volume	19	58.668	8.506	0.934	0.0001	*significant*

Table 13: Statistical framework for the linear QSPR model for $ABC(G)$

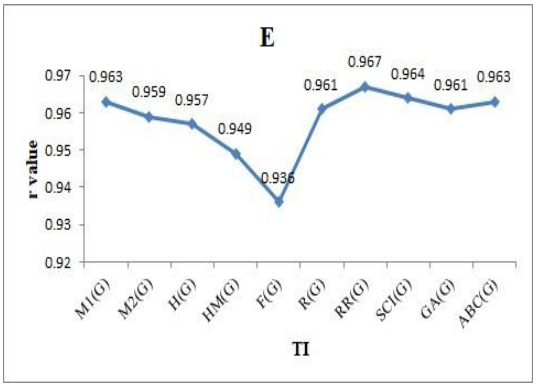
Physical Properties	**N**	**a**	**b**	**r**	**p**	**Indicator**
BoilingPoint	17	233.037	17.747	**0.97**	0.0001	*significant*
Enthalpy	17	46.588	2.295	0.965	0.0001	*significant*
FlashPoint	17	50.338	12.522	0.946	0.0001	*significant*
logP	19	−3.495	0.29	0.875	0.0001	*significant*
Molar Volume	19	41.905	12.315	0.949	0.0001	*significant*

Table 14: Correlation coefficient values of Physico-chemical properties of Asthma Drugs with Topological indices

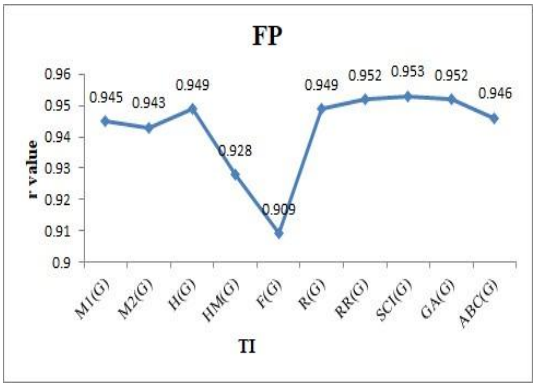
Index	Boiling Point	Enthalpy	Flash Point	logP	Molar Volume
$M_1(G)$	0.97	0.963	0.945	**0.882**	0.921
$M_2(G)$	0.966	0.959	0.943	0.879	0.894
$H(G)$	0.964	0.957	0.949	0.855	0.965
$HM(G)$	0.954	0.949	0.928	0.880	0.887
$F(G)$	0.941	0.936	0.909	0.877	0.877
$R(G)$	0.967	0.961	0.949	0.861	**0.966**
$RR(G)$	**0.974**	**0.967**	0.952	0.881	0.924
$SCI(G)$	0.971	0.964	**0.953**	0.867	0.958
$GA(G)$	0.968	0.961	0.952	0.864	0.934
$ABC(G)$	0.97	0.965	0.946	0.875	0.949



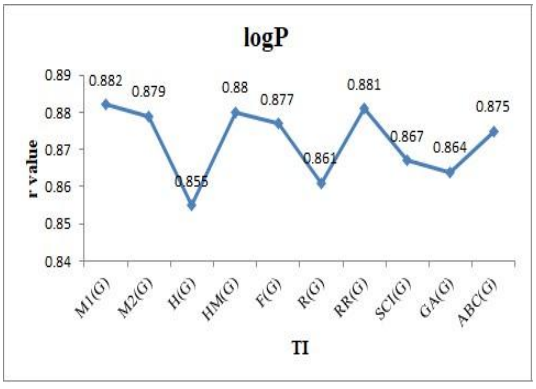
(a) TI on BP



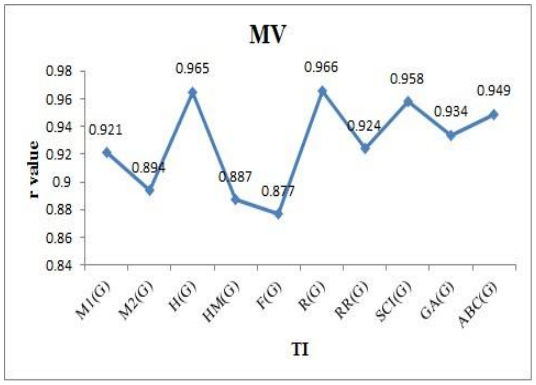
(b) TI on E



(c) TI on FP



(d) TI on logP



(e) TI on MV

Figure 2: Physico-chemical properties of Various Asthma Drugs with Topological indices

5. RESULTS AND DISCUSSION

From the above results, it is noticed that the Reciprocal Randic index gives high correlation coefficient value 0.974 and 0.967 for the Boiling Point and Enthalpy respectively. Also Sum connectivity index gives 0.953 for Flash Point, First zagreb index gives 0.882 for logP and Randic index gives 0.996 for Molar Volume of defined ten topological indices for five physico- chemical properties.

6. CONCLUSION

Topological indices are the numerical descriptors used to analyse the physical and chemical characteristics of chemical compounds. The various topological indices values are computed for asthma drugs. Also QSPR study is carried out on these drugs, which helps in finding the characteristics of drugs without conducting any experiment which is time consuming. It may help the chemists to design drug for the treatment of Covid-19 in the pandemic situation, because of Covid-19 most of the people are dying who have respiratory problems (asthma).

ACKNOWLEDGMENT

The Authors would like to thank the reviewers for their helpful suggestions and comments. The authors are thankful to
Dr. Preethi K.R. for her valuable suggestions.

7. REFERENCES

[1] Adnan Aslam, Safyan Ahmad and Wei Gao, On Topological Indices of Boron Triangular Nanotubes, *Z. Naturforsch.* **2017**, *72(8)*, 711-716.

[2] Anil Kumar K.N., Basavarajappa N.S., Shanmukha M.C., QSPR analysis of Alkanes with certain degree based topological indices, *Malaya Journal of Mathematik* **2020,** *8(1)*, 314-330.

[3] Estrada E.; Torres L., Rodriguez L., Gutman I., An atom-bond connectivity index: Modeling the enthalpy of formation of alkanes, *Indian J. Chem.* **1998**, *37(A)*, 849-855.
[4] Fajtlowicz S., On Conjectures of Grafitti II, *Congr. Number.* **1987**, *60*, 189-197.
[5] Favaron O.; Maheo M. and J.F. Sacle, Some eigenvalue properties in graphs (conjectures of graffiti-II), *Discrete Math* **1993**, *111(1-3)*, 197-220.
[6] Furtula B. and Gutman I, A forgotton topological index, *J. Math. Chem.* **2015,** *53*, 213-220.
[7] Gutman I., Degree Based Topological Indices, *Croat. Chem. Acta* **2013**, *86*, 351-361.
[8] Hosamani S. M., Deepa Perigidad, Shruti Jamagoud Yallavva Maled and Sharada Gavade, QSPR Analysis of Certain Degree Based Topological Indices, *Journal of Statistics Applications and Probability* **2017**, *6(2)*, 1-11.
[9] Randic M., On Characterization of molecular branching, *J. Amer. Chem. Soc.* **1975**, *97*, 6609-6615.
[10] Randic M., Comparative structure-property studies: Regressions using a single descriptor. *Croat. Chem. Acta* **1993**, *66*, 289-312.
[11] Randic M., Quantitative Structure-Property Relationship: boiling points and planar benzenoids, *New. j. Chem.* **1996**, *20*, 1001-1009.
[12] Shanmukha M. C., Basavarajappa N. S. and Anil Kumar K. N., Predicting physicochemical properties of octane isomers using QSPR approach, *Malaya Journal of Mathematik* **2020**, *8 (1)*, 104-116.
[13] Shanmukha M.C., Basavarajappa N.S., A. Usha and Shilpa K C., Novel Neighbourhood redefined First and Second Zagreb indices on Carborundum Structures, *Journal of Applied Mathematics and Computing*, **2020**, p. 1-14.
[14] DOI: 10.1007/s12190-020-01435-3.
[15] Shirdel G. H., RezaPour H., Sayadi A. M., The Hyper-Zagreb Index of Graph Operations. *Iranian Journal of Mathematical Chemistry* **2013**, *4(2)*, 213-220.
[16] Stacy Gelhaus Wendell, Hao Fan and Cheng Zhang, G Protein-Coupled Receptors in Asthma Therapy: Pharmacology and Drug Action, *Pharmacological Reviews* **2020**, *72*, 1-49.
[17] Vukicevic D., Furtula B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem*. **2009**, *46*, 1369-1376.
[18] Zhou B. and Trinajstic N., On general sum-connectivity index, *J. Math. Chem.* **2010**, *47*, 210-218.
[19] Shanmukha M.C., Basavarajappa N.S. Anil Kumar K.N. and A. Usha, Degree-Based Topological Indices of Dox-loaded Peg-Pasp Polymer, *Jñānābha*, **2020,** *50(1)*, 89-101.
[20] Shanmukha M.C., Basavarajappa N.S., Shilpa K C. and A. Usha , Erratum to Degree-based topological indices on anticancer drugs with QSPR analysis, *Heliyon*, **2020**, *6*, 1-9.