Fuzzy Systems and Soft Computing
ISSN : 1819-4362

DEGREE BASED MOLECULAR DESCRIPTORS AND QSPRANALYSIS OF HYPERTENSION BETA BLOCKER DRUGS

Dr.G.Priyadharsini Assistant Professor, Kongu Arts and Science Colleg e(Autonomous),Erode–638107
Ms. V. Amudhamalar Assistant Professor,VET Institute of Arts and Science (Co-education) College, Erode–638012
Mr. P.Sathish Assistant Professor, Nandha Arts and Science College, Erode–638052

Abstract:
Thisstudydescribingfocusesonexploringthequantitativestructure-propertyrelationship(QSPR)ofsixhypertensive medications. QSPR is a method used in computational chemistry to correlate the molecular structure of compounds with their physical, chemical, or biological properties. In this case, the properties of interest are likely related to the efficacy or pharmacological behavior of the hypertensive drugs.

Keywords:QSPR,TopologicalIndices,Molecularstructures.SubjectClassification:05C92

1. Introduction:

Hypertension,commonlyknownas highblood pressure,referstoa conditionwheretheforce oftheblood againstthe wallsofthearteriesisconsistentlytoohigh.Thisconditionisasignificanthealthconcernbecauseitcanleadtoserious health problems over time, such as heart disease, stroke, and damage to other organs. Bloodpressureismeasuredusingtwonumbers:

Therearetwomaintypesofhypertension:

- Primary (essential) hypertension: This is the most common type and develops gradually over many years withoutanyidentifiablecause.Ittendstodevelopovertimeduetoacombinationoffactorsincludinggenetics, lifestyle choices (such as diet and physical activity), and environmental factors.
- Secondary hypertension: This type of hypertension is caused by an underlying condition, such as kidney disease, hormonal disorders, certain medications, or other health problems.

Managing hypertensiontypically involves lifestyle changes suchas adopting a healthydiet (low insalt, rich in fruits and vegetables),regularexercise,maintaininga healthyweight, limitingalcoholconsumption,andquittingsmoking. In some cases, medication may also be necessaryto control blood pressure effectively. Regular monitoring of blood pressure is crucial because hypertension often does not cause symptoms initially but can still cause damage to the cardiovascular system and other organs over time if left untreated.Hypertension, or high blood pressure, often does notcausenoticeablesymptoms,whichiswhyitiscommonlyreferredtoasa"silentkiller."However,whensymptoms do occur, they can include:

1. Headaches:Oftensevereandoccurringinthemorning.
2. ShortnessofBreath:Difficultybreathing,especiallyduringphysicalactivities.
3. Nosebleeds:Morefrequentandunexplained.
4. ChestPain:Pain,pressure,ortightnessinthechest.
5. Dizziness:Feelinglightheadedor faint.
6. VisualChanges:Blurred ordouble vision.
7. Fatigue:Unusualtirednessor lackofenergy.
8. IrregularHeartbeat:Palpitationsoraflutteringsensationinthechest.
9. BloodintheUrine:Haematuria,thoughthisisless common.

10. Confusion:Severecasescanleadtoconfusionordifficultyconcentrating.

1.1 Non-ModifiableRiskFactors
1. Age:Riskincreaseswithage.
2. FamilyHistory:Afamilyhistoryofhypertensionincreasestherisk.
3. Ethnicity:Certainethnicgroups,suchasAfricanAmericans,areat higherrisk.
4. Gender:Menaregenerallyathigherriskthanwomenuntilage64,afterwhichtheriskforwomenincreases.

1.2 ModifiableRisk Factors
1. Diet:Highsalt(sodium) intake, lowpotassiumintake,and diets highinsaturated fatsand cholesterolcan increase risk.
2. PhysicalInactivity:Lackofregularphysicalactivitycanleadtoweightgainandhigherbloodpressure
3. Weight:Overweightandobesitysignificantlyincreasetherisk.
4. AlcoholConsumption:Excessivealcohol intakecanraiseblood pressure.
5. TobaccoUse:Smoking orchewingtobaccoimmediatelyraisesbloodpressureanddamagesthelining of your artery walls.
6. Stress:Highlevelsofstresscanleadtoa temporaryincrease inblood pressure.
7. ChronicConditions:Conditionssuchasdiabetes,kidneydisease,andsleepapneacanincreaserisk.
8. Medications:Certainmedications,suchasbirthcontrolpills,coldremedies,and over-the-counterpain relievers, can increase blood pressure.

Hypertension,orhighbloodpressure,iscategorizedintodifferentstagesbasedonsystolicanddiastolicblood pressure readings. The American College of Cardiology (ACC) and the American Heart Association (AHA) define the following blood pressure categories:

1.3 BloodPressureCategories
1. NormalBloodPressure:
o Systolic:Lessthan120mmHg
o Diastolic:Lessthan80mmHg
2. ElevatedBloodPressure:
o Systolic:120-129mmHg
o Diastolic:Lessthan80mmHg
3. HypertensionStage 1:
o Systolic:130-139mmHg
o Diastolic:80-89 mmHg
4. HypertensionStage 2:
o Systolic:140mmHgor higher
o Diastolic:90mmHgorhigher
5. HypertensiveCrisis(requiresimmediatemedicalattention):
o Systolic:Higherthan180mmHg
o Diastolic:Higherthan120mmHg
o

2. Topologicalindexsignificanceand Applications:
Topologicalindicesarenumericalvaluesassociatedwiththestructureofamolecule,derivedfromitsgraph-theoretical properties. These indices play a crucial role in the study of chemical graph theory and molecular chemistry. They provide insightsintothemolecularstructure,properties,andbehaviour,whichareessentialforvariousapplicationsin chemistry, pharmacology, and materials science.

Methods:

Several methodologies, including QSAR, QSPR, and QSTR, allow chemists or pharmacists to use drug-related data,suchas meltingpoint, boiling point, molarrefractivity, density, enthalpy, vaporization, flashpoint,polarsurface area, polarizability, molar volume, and so on, for further research and novel medication design. QSPR analysis provides a systematic method for discovering the qualities of drugs that contribute to their effectiveness in treating variousaspectsofthisailment.DrugselectionforQSPRanalysisbasedontopologicalindicestakesintoaccountboth the drug's attributes and the required properties.

The availability of a data set of medications or compounds that includes both structural information (needed for generating topological indices) and property values influences the choice of a drug. The medicinal molecule should have a well-defined chemical structure and atomic connectivity. In QSPR analysis of medications for hypertension treatment, beta blockers are discussed using topological indices. We demonstrate that the qualities obtained from associated topological indices and the physical properties of the recognized medications are substantially connected using linear regression. Molecular graphs of pharmaceuticals are used to simulate the problem in chemical graph theory; atoms correspond to the graph's vertices, and edges represent the bonds between two atoms. Consider G (V, E), a molecular graph with vertex and edge sets denoted byV and E, respectively.

Definition:1.1:ThefirstandsecondZagrebindicesareamongtheprimitiveindicesdesignedbyTrinajsticand Gutman, which are defined as [1]

$$M_1(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}(\delta_a+\delta_b),$$
$$M_2(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}(\delta_a\delta_b)$$

Definition:1.2: HarmonicIndexisgivenby[7]

$$(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\frac{2}{(\delta_a+\delta_b)}$$

Definition:1.3: RandicIndexintroduced[5]

$$(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\frac{1}{\sqrt{(\delta_a\delta_b)}}$$

Definition:1.4: EstradaIndexintroduced [2]

$$ABC(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\sqrt{\frac{\delta_a+\delta_b-2}{\delta_a\delta_b}}$$

Definition:1.5: Vukicevicet al[3]introduced Inverse IndegIndexas

$$IS(\mathbb{G})=\sum_{e\epsilon E(H)}\frac{\delta_a\delta_b}{\delta_a+\delta_b}$$

Definition:1.6: Zhaoetal.[4]formulated theSSindexwhichisdefinedas

$$SS(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\sqrt{\frac{\delta_a\delta_b}{\delta_a+\delta_b}}$$

Definition:1.7: Gutmanformulatedthesombor indexwhichisdefinedas

$$(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\sqrt{(\delta_a)^2+(\delta_b)^2}$$

Definition:1.8: ReciprocalRandicIndexintroduced[6]

$$RR(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\sqrt{(\delta_a\delta_b)}$$

Definition:1.9: HyperZagrebIndex

$$(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\frac{2}{\delta_a+\delta_b}$$

Definition:1.10: AugmentedZagrebIndex

$$A(\mathbb{G})=\sum_{e\epsilon E(\mathbb{G})}\left(\frac{\delta_a\delta_b}{\delta_a+\delta_b-2}\right)^3$$

Definition:1.11: ForgottenIndexintroduced[26]

$$(\mathbb{G})=\sum_{e\epsilon(\mathbb{G})}(\delta_a)^2+(\delta_b)^2$$

Definition:1.12: GeometricArithmeticintroduced[10]

$$(\mathfrak{G})=\sum_{e\epsilon E(\mathfrak{G})} \frac{\delta_a+\delta_b}{\delta_a+\delta_b}$$

Definition:1.13: SumConnectivity

$$(\mathfrak{G})=\sum_{e\epsilon E(\mathfrak{G})} \frac{1}{\sqrt{(\delta_a+\delta_b)}}$$

Definition:1.14: RedefinedZagreb Index

$$ReZ(\mathfrak{G})=\sum_{e\epsilon E(\mathfrak{G})} \frac{\delta_a+\delta_b}{\delta_a\delta_b}$$

TABLE :1 COMPUTED VALUES OF TI's FOR HYPER TENSION BETA BLOCKER DRUGS

DrugName	M_1	M_2	HH	ABC	IS	SS	AZI	SO	R	RR	H	F	GA	SC	ReZ
Nadolol	97	110	463	15.05	22.88	21.76	58.03	70.45	9.8	47.1	9.63	243	20.3	9.9	20.5
Propranolol	92	103	432	14.39	21.85	20.81	54.7	66.61	9.2	44.8	8.87	226	19.44	9.4	19
Atenolol	86	91	394	13.98	19.75	19.28	128.9	63.18	8.8	41.2	8.5	212	18.13	8.9	19
Metoprolol	84	89	378	15.55	19.72	19.27	47.2	61.43	9.1	40.7	8.76	200	15.36	9.1	19
Carvedilol	153	177	727	23.28	37.22	34.92	272.9	109.6	14.8	75.5	14.59	373	32.5	15.5	33.88
Labetalol	113	124	523	18.03	26.67	25.68	188.3	82.05	11.8	54.8	11.3	275	23.8	11.9	26.65

TABLE :2 PHYSICO CHEMICALPROPERTIESOFHYPERTENSIONBETABLOCKERDRUGS

DrugName	D	BP	VP	E	FP	IR	MR	PSA	P	ST	MV
Nadolol	1.2	526	1.5	84.3	272.2	1.57	85.8	82	34	46.6	260
Propranolol	1.1	435	1.1	73	217	1.6	79	41	31	43	237
Atenolol	1.1	508	1.4	81.9	261.1	1.54	74.3	85	29.4	45.6	236.7
Metoprolol	1.0	398.6	1.0	68.5	194.9	1.51	77.1	51	37	30.6	258.7
Carvedilol	1.3	655.2	2.1	101.4	350.1	1.65	119.6	76	47	53.9	325.1
Labetalol	1.2	552.7	1.6	87.7	288.1	1.61	94.7	96	37.6	55.1	273.6

TABLE:3 StatisticalSpecificationsfortheLinearModelof $M_1(\mathfrak{G})$

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.784	0.004	0.874	0.764	12.943	0.570
BP	6	189.3	3.104	0.892	0.795	15.547	45.889
VP	6	0.011	0.014	0.915	0.837	20.515	0.1778
E	6	40.972	0.402	0.902	0.814	17.464	5.6019
FP	6	68.468	1.876	0.891	0.795	15.488	27.793
IR	6	1.394	0.002	0.881	0.776	13.869	0.0283
MR	6	21.105	0.646	0.995	0.989	365.36	1.971
PSA	6	44.245	0.265	0.325	0.105	0.471	22.497
P	6	13.744	0.214	0.887	0.787	14.792	3.24
ST	6	20.351	0.243	0.716	0.513	4.217	6.91
MV	6	141.875	1.184	0.945	0.894	33.589	11.911

TABLE4 StatisticalSpecificationsfortheLinearModelof $M_2(\mathfrak{G})$

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.8210	0.003	0.887	0.786	14.706	0.0542
BP	6	228.13	2.460	0.886	0.785	14.616	47.022
VP	6	0.1840	0.011	0.909	0.826	19.043	0.183
E	6	45.983	0.318	0.897	0.804	16.38	5.75
FP	6	91.922	1.487	0.886	0.785	14.579	28.46
IR	6	1.4130	0.001	0.894	0.800	15.989	0.0267
MR	6	28.910	0.514	0.993	0.986	276.94	2.26
PSA	6	49.740	0.191	0.294	0.806	0.377	22.7369
P	6	23.397	0.193	0.712	0.507	4.106	6.9559
ST	6	16.540	0.168	0.876	0.767	13.166	3.389
MV	6	156.95	0.936	0.937	0.937	0.878	28.757

TABLE5 StatisticalSpecificationsfortheLinearModelofHM(Ꮆ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.797	0.001	0.893	0.798	15.764	0.053
BP	6	205.342	0.632	0.898	0.806	16.572	44.731
VP	6	0.085	0.003	0.919	0.845	21.779	0.1734
E	6	43.064	0.082	0.907	0.823	18.654	5.453
FP	6	78.148	0.382	0.897	0.805	16.525	27.082
IR	6	1.401	0.000	0.894	0.799	15.885	0.0268
MR	6	24.955	0.131	0.993	0.986	281.3	2.243
PSA	6	46.254	0.053	0.319	0.102	0.452	22.54
P	6	15.356	0.042	0.871	0.759	12.63	3.443
ST	6	21.432	0.050	0.726	0.527	4.465	6.81
MV	6	149.5	0.237	0.937	0.877	28.601	12.793

TABLE6 StatisticalSpecificationsfortheLinearModelofABC(Ꮆ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.774	0.023	0.759	0.576	5.4322	0.076
BP	6	165.81	20.775	0.810	0.656	7.622	59.124
VP	6	-0.121	0.094	0.846	0.715	10.042	0.235
E	6	37.73	2.7	0.823	0.677	8.384	7.375
FP	6	54.342	12.55	0.809	0.655	7.589	36.04
IR	6	1.386	0.012	0.776	0.602	0.061	0.037
MR	6	10.20	4.686	0.978	0.957	89.289	3.921
PSA	6	44.83	1.62	0.269	0.072	0.312	22.91
P	6	7.51	1.71	0.962	0.925	48.991	1.93
ST	6	21.375	1.457	0.582	0.339	2.048	8.0525
MV	6	113.78	9.071	0.982	0.964	108.58	6.884

TABLE7 StatisticalSpecificationsfortheLinearModelofIS(Ꮆ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.813	0.014	0.866	0.750	12.027	0.0586
BP	6	216.95	11.98	0.878	0.772	13.522	48.4681
VP	6	0.131	0.053	0.903	0.816	17.692	0.1890
E	6	44.514	1.551	0.889	0.791	15.131	5.934
FP	6	85.185	7.241	0.878	0.771	13.476	29.35
IR	6	1.407	0.007	0.882	0.778	14.045	0.0281
MR	6	25.914	2.532	0.995	0.990	379.71	1.9377
PSA	6	48.677	0.938	0.293	0.086	0.377	22.737
P	6	15.215	0.842	0.893	0.797	15.662	3.1663
ST	6	22.744	0.930	0.699	0.488	3.818	7.0828
MV	6	150.382	4.651	0.948	0.898	35.129	11.6770

TABLE8 StatisticalSpecificationsfortheLinearModelofSO(Ꮆ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.769	0.005	0.875	0.766	13.072	0.056
BP	6	175.4	4.46	0.896	0.803	16.335	44.99
VP	6	-0.050	0.020	0.919	0.844	21.678	0.173
E	6	39.189	0.577	0.906	0.821	18.376	5.486
FP	6	60.078	2.698	0.896	0.803	16.269	27.25
IR	6	1.387	0.003	0.878	0.770	13.423	0.028
MR	6	18.576	0.924	0.994	0.989	353.0	2.0046
PSA	6	42.05	0.394	0.338	0.114	0.515	22.388
P	6	12.908	0.306	0.887	0.787	14.761	3.2414
ST	6	19.225	0.350	0.721	0.520	4.330	6.862
MV	6	139.966	1.697	0.947	0.896	34.528	11.7678

TABLE9 StatisticalSpecificationsfortheLinearModelofSS(Ꮆ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.795	0.015	0.861	0.741	11.415	0.0597
BP	6	198.735	13.290	0.880	0.775	13.794	48.0954
VP	6	0.050	0.059	0.905	0.819	18.125	0.1872
E	6	42.164	1.721	0.891	0.794	15.433	5.8874
FP	6	74.183	8.034	0.880	0.775	13.741	29.1289
IR	6	1.389	0.008	0.874	0.765	12.988	0.03
MR	6	22.192	2.804	0.995	0.990	404.35	1.8744
PSA	6	45.911	1.098	0.310	0.096	0.426	22.612
P	6	13.844	0.938	0.898	0.807	16.694	3.0864
ST	6	21.318	1.032	0.701	0.491	3.859	7.0643
MV	6	143.1	5.171	0.951	0.905	38.260	11.2362

TABLE 10 StatisticalSpecificationsfortheLinearModelofAZI(Ꮾ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	1.038	0.001	0.775	0.601	6.035	0.07440
BP	6	400.698	0.895	0.898	0.806	16.571	44.732
VP	6	0.962	0.004	0.903	0.815	17.679	0.1891
E	6	68.425	0.115	0.901	0.813	17.344	5.6176
FP	6	196.296	0.541	0.897	0.804	16.426	27.1475
IR	6	1.526	0.000	0.752	0.566	5.212	0.0394
MR	6	68.260	0.161	0.866	0.750	12.003	9.4686
PSA	6	55.81	0.128	0.548	0.301	1.719	19.892
P	6	29.626	0.051	0.739	0.546	4.810	4.7301
ST	6	36.31	0.075	0.772	0.596	5.896	6.953
MV	6	228.581	0.293	0.816	0.665	7.944	21.135

TABLE 11 StatisticalSpecificationsfortheLinearModelofR(Ꮾ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.742	0.038	0.849	0.720	10.307	0.062
BP	6	145.488	34.582	0.884	0.781	14.26	47.48
VP	6	-0.187	0.154	0.908	0.825	18.80	0.184
E	6	35.322	4.473	0.893	0.798	15.828	5.8284
FP	6	42.017	20.90	0.883	0.780	14.192	28.766
IR	6	1.375	0.019	0.844	0.712	9.891	0.0321
MR	6	11.458	7.250	0.992	0.985	256.875	2.345
PSA	6	35.305	3.441	0.375	0.141	0.655	22.0486
P	6	9.755	2.417	0.913	0.833	20.023	2.8645
ST	6	16.959	2.71	0.709	0.502	4.038	6.9851
MV	6	121.384	13.546	0.961	0.924	48.965	10.0366

TABLE 12 StatisticalSpecificationsfortheLinearModelofRR(Ꮾ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.800	0.007	0.870	0.757	12.436	0.0578
BP	6	204.253	6.087	0.885	0.783	14.416	47.28
VP	6	0.076	0.027	0.909	0.826	18.944	0.1838
E	6	42.887	0.788	0.895	0.802	16.162	5.7799
FP	6	77.510	3.680	0.884	0.782	14.365	28.63
IR	6	1.401	0.004	0.882	0.777	43.948	0.0282
MR	6	23.693	1.278	0.995	0.990	380.7	1.9312
PSA	6	46.716	0.496	0.307	0.094	0.417	22.633
P	6	14.532	0.424	0.890	0.792	15.273	3.1981
ST	6	21.666	0.475	0.71	0.499	3.987	7.01
MV	6	146.366	2.346	0.947	0.897	34.765	11.7317

TABLE 13 StatisticalSpecificationsfortheLinearModelofH(Ꮾ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.757	0.038	0.855	0.731	10.888	0.0608
BP	6	162.331	34.08	0.881	0.776	13.859	48.01
VP	6	-0.115	0.152	0.907	0.823	18.540	0.1854
E	6	37.473	4.411	0.891	0.794	15.438	5.8866
FP	6	52.182	20.60	0.881	0.775	13.803	29.078
IR	6	1.383	0.019	0.847	0.717	10.157	0.0318
MR	6	14.389	7.204	0.997	0.995	727.77	1.4002
PSA	6	39.073	3.188	0.351	0.123	0.564	22.267
P	6	10.718	2.46	0.919	0.844	21.685	2.7703
ST	6	18.695	2.628	0.696	0.484	3.754	7.112
MV	6	126.697	13.477	0.967	0.936	58.458	9.2424

TABLE 14 StatisticalSpecificationsfortheLinearModelofF(Ꞵ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.772	0.001	0.899	0.808	16.841	0.0514
BP	6	181.95	1.297	0.909	0.825	18.912	42.385
VP	6	-0.017	0.006	0.929	0.862	25.089	0.1632
E	6	40.070	0.168	0.918	0.842	21.392	5.1504
FP	6	64.008	0.784	0.908	0.825	18.850	25.67
IR	6	1.390	0.001	0.892	0.796	15.64	0.027
MR	6	21.002	0.265	0.992	0.984	253.37	2.361
PSA	6	42.454	0.115	0.344	0.119	0.538	22.33
P	6	14.184	0.086	0.866	0.750	12.024	3.51
ST	6	19.391	0.103	0.741	0.549	4.859	6.653
MV	6	142.717	0.481	0.935	0.874	27.661	12.98

TABLE 15 StatisticalSpecificationsfortheLinearModelofSC(Ꞵ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.770	0.035	0.848	0.719	10.251	0.0621
BP	6	172.58	31.53	0.878	0.771	13.489	48.51
VP	6	-0.068	0.141	0.904	0.816	17.787	0.1886
E	6	38.788	4.081	0.889	0.790	15.029	5.9495
FP	6	58.391	19.058	0.878	0.771	13.429	29.3883
IR	6	1.387	0.018	0.856	0.732	10.931	0.0309
MR	6	16.533	6.667	0.995	0.989	362.35	1.9790
PSA	6	41.269	2.834	0.337	0.113	0.511	22.3958
P	6	11.585	2.264	0.911	0.831	19.599	2.8901
ST	6	19.343	2.44	0.697	0.486	3.789	7.0960
MV	6	131.390	12.41	0.960	0.921	46.895	10.2386

TABLE 16 StatisticalSpecificationsfortheLinearModelofRE(Ꞵ)

Physical Properties	n	γ	δ	r	r^2	F	S.E
D	6	0.817	0.014	0.841	0.707	9.664	0.0634
BP	6	209.612	13.169	0.885	0.784	14.491	47.180
VP	6	0.102	0.059	0.907	0.824	18.669	0.1849
E	6	43.647	1.702	0.894	0.800	15.977	5.8066
FP	6	80.788	7.959	0.885	0.783	14.41	28.59
IR	6	1.413	0.007	0.837	0.701	9.395	0.033
MR	6	25.558	2.732	0.984	0.968	120.14	3.3996
PSA	6	39.390	1.410	0.404	0.163	0.782	21.754
P	6	14.610	0.930	0.903	0.816	17.699	3.014
ST	6	21.538	1.050	0.723	0.523	4.387	6.838
MV	6	147.896	5.098	0.952	0.906	38.58	11.1936

TABLE 17 CorrelationcoefficientbetweenphysicochemicalpropertiesandTI'sofHypertensionBetaBlockerDrugs

Index	M_1 (Ꞵ)	M_2 (Ꞵ)	HM (Ꞵ)	ABC (Ꞵ)	IS (Ꞵ)	SO (Ꞵ)	SS (Ꞵ)	AZI (Ꞵ)	R (Ꞵ)	RR (Ꞵ)	H (Ꞵ)	F (Ꞵ)	GA (Ꞵ)	SC (Ꞵ)	REG (Ꞵ)
D	0.874	0.887	0.893	0.759	0.866	0.875	0.861	0.775	0.849	0.870	0.855	0.899	0.919	0.848	0.841
BP	0.892	0.886	0.898	0.810	0.878	0.896	0.880	0.898	0.884	0.885	0.881	0.909	0.924	0.878	0.885
VP	0.915	0.909	0.919	0.846	0.903	0.919	0.905	**0.903**	0.908	0.909	0.907	0.929	0.937	0.904	0.907
E	0.902	0.897	0.907	0.823	0.889	0.906	0.891	0.901	0.893	0.895	0.891	0.918	0.932	0.889	0.894
FP	0.891	0.886	0.897	0.809	0.878	0.896	0.880	0.897	0.883	0.884	0.881	0.908	0.924	0.878	0.885
IR	0.881	0.894	0.894	0.776	0.882	0.878	0.874	0.752	0.844	0.882	0.847	0.892	0.923	0.856	0.837
MR	**0.995**	**0.993**	**0.993**	**0.978**	**0.995**	**0.994**	**0.995**	0.866	**0.992**	**0.995**	**0.997**	**0.992**	**0.975**	**0.995**	**0.984**
PSA	0.325	0.294	0.319	0.269	0.293	0.338	0.310	0.548	0.375	0.307	0.351	0.344	0.371	0.337	0.404
P	0.887	0.712	0.871	0.962	0.893	0.887	0.898	0.739	0.913	0.890	0.919	0.866	0.812	0.911	0.903
ST	0.716	0.876	0.726	0.582	0.699	0.721	0.701	0.772	0.709	0.71	0.696	0.741	0.795	0.697	0.723
MV	0.945	0.937	0.937	0.982	0.948	0.947	0.951	0.816	0.961	0.947	0.967	0.935	0.894	0.960	0.952

1.3.RegressionModels

Thelinearregressionmodelisgivenby

$P=\gamma+(TI)$ (A)

whereP,γ, δ, TI⟶physicalpropertyofdrug, constant,regressioncoefficient, and topologicalindex. Usingequation(A),thelinearmodelsfortherespectivetopologicalindicesconsideredinthestudyareobtained as follows.

FirstZagrebindex$M_1(H)$:

D	=	0.784	+	0.004	$[M_1(G)]$
BP	=	189.3	+	3.104	$[M_1(G)]$
VP	=	0.011	+	0.014	$[M_1(G)]$
E	=	40.972	+	0.402	$[M_1(G)]$
FP	=	68.468	+	1.876	$[M_1(G)]$
IR	=	1.394	+	0.002	$[M_1(G)]$
MR	=	21.105	+	0.646	$[M_1(G)]$
PSA	=	44.245	+	0.265	$[M_1(G)]$
P	=	13.744	+	0.214	$[M_1(G)]$
ST	=	20.351	+	0.243	$[M_1(G)]$
MV	=	141.875	+	1.184	$[M_1(G)]$

SecondZagrebindex$M_2(G)$:

D	=	0.8210	+	0.003	$[M_2(G)]$
BP	=	228.13	+	2.460	$[M_2(G)]$
VP	=	0.1840	+	0.011	$[M_2(G)]$
E	=	45.983	+	0.318	$[M_2(G)]$
FP	=	91.922	+	1.487	$[M_2(G)]$
IR	=	1.4130	+	0.001	$[M_2(G)]$
MR	=	28.910	+	0.514	$[M_2(G)]$
PSA	=	49.740	+	0.191	$[M_2(G)]$
P	=	23.397	+	0.193	$[M_2(G)]$
ST	=	16.540	+	0.168	$[M_2(G)]$
MV	=	156.95	+	0.936	$[M_2(G)]$

HyperZagrebIndexHM(G)

D	=	0.797	+	0.001	[HM(G)]
BP	=	205.342	+	0.632	[HM(G)]
VP	=	0.085	+	0.003	[HM(G)]
E	=	43.064	+	0.082	[HM(G)]
FP	=	78.148	+	0.382	[HM(G)]
IR	=	1.401	+	0.000	[HM(G)]
MR	=	24.955	+	0.131	[HM(G)]
PSA	=	46.254	+	0.053	[HM(G)]
P	=	15.356	+	0.042	[HM(G)]
ST	=	21.432	+	0.050	[HM(G)]
MV	=	149.5	+	0.237	[HM(G)]

InverseindegindexIS(G):

D	=	0.813	+	0.014	[IS(G)]
BP	=	216.95	+	11.98	[IS(G)]
VP	=	0.131	+	0.053	[IS(G)]
E	=	44.514	+	1.551	[IS(G)]
FP	=	85.185	+	7.241	[IS(G)]
IR	=	1.407	+	0.007	[IS(G)]
MR	=	25.914	+	2.532	[IS(G)]
PSA	=	48.677	+	0.938	[IS(G)]
P	=	15.215	+	0.842	[IS(G)]
ST	=	22.744	+	0.930	[IS(G)]
MV	=	150.382	+	4.651	[IS(G)]

AugmentedZagrebIndex AZI(G):

D	=	1.038	+	0.001	[AZI(G)]
BP	=	400.698	+	0.895	[AZI(G)]
VP	=	0.962	+	0.004	[AZI(G)]
E	=	68.425	+	0.115	[AZI(G)]
FP	=	196.296	+	0.541	[AZI(G)]
IR	=	1.526	+	0.000	[AZI(G)]
MR	=	68.260	+	0.161	[AZI(G)]
PSA	=	55.81	+	0.128	[AZI(G)]
P	=	29.626	+	0.051	[AZI(G)]
ST	=	36.31	+	0.075	[AZI(G)]
MV	=	228.581	+	0.293	[AZI(G)]

EstradaIndexABC (G)

D	=	0.774	+	0.023	[ABC(G)]
BP	=	165.81	+	20.775	[ABC(G)]
VP	=	-0.121	+	0.094	[ABC(G)]
E	=	37.73	+	2.7	[ABC(G)]
FP	=	54.342	+	12.55	[ABC(G)]
IR	=	1.386	+	0.012	[ABC(G)]
MR	=	10.20	+	4.686	[ABC(G)]
PSA	=	44.83	+	1.62	[ABC(G)]
P	=	7.51	+	1.71	[ABC(G)]
ST	=	21.375	+	1.457	[ABC(G)]
MV	=	113.78	+	9.071	[ABC(G)]

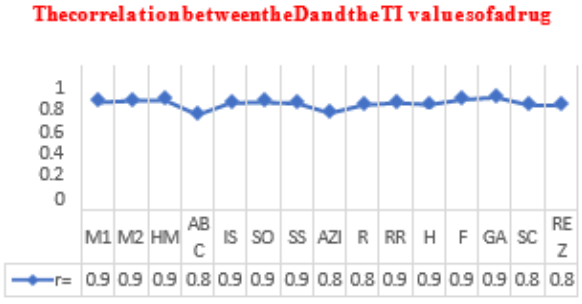
SomberindexSO(G):

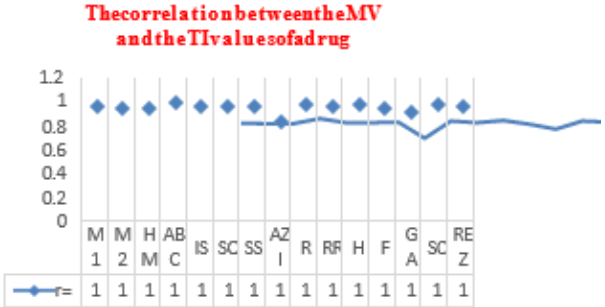
D	=	0.769	+	0.014	[SO(G)]
BP	=	175.4	+	11.98	[SO(G)]
VP	=	-0.050	+	0.053	[SO(G)]
E	=	39.189	+	1.551	[SO(G)]
FP	=	60.078	+	7.241	[SO(G)]
IR	=	1.387	+	0.007	[SO(G)]
MR	=	18.576	+	2.532	[SO(G)]
PSA	=	42.05	+	0.938	[SO(G)]
P	=	12.908	+	0.842	[SO(G)]
ST	=	19.225	+	0.930	[SO(G)]
MV	=	139.966	+	4.651	[SO(G)]

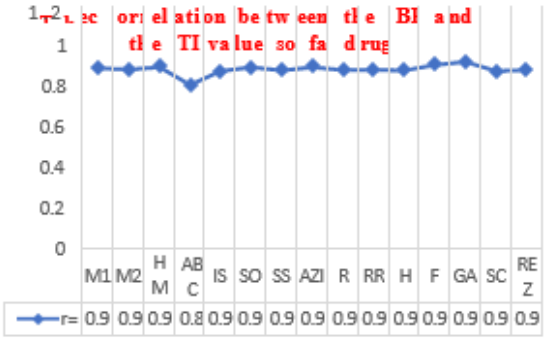
SSindexSS(G):

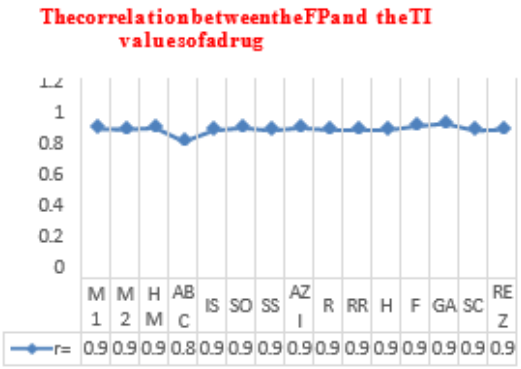
D	=	0.795	+	0.015	[SS(G)]
BP	=	198.735	+	13.290	[SS(G)]
VP	=	0.050	+	0.059	[SS(G)]
E	=	42.164	+	1.721	[SS(G)]
FP	=	74.183	+	8.034	[SS(G)]
IR	=	1.389	+	0.008	[SS(G)]
MR	=	22.192	+	2.804	[SS(G)]
PSA	=	45.911	+	1.098	[SS(G)]
P	=	13.844	+	0.938	[SS(G)]
ST	=	21.318	+	1.032	[SS(G)]
MV	=	143.1	+	5.171	[SS(G)]

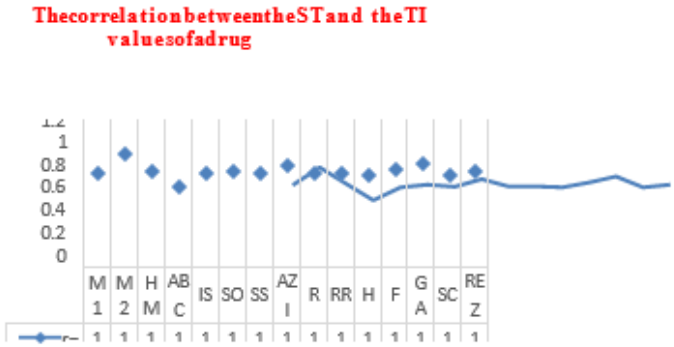
GraphAnalysis:

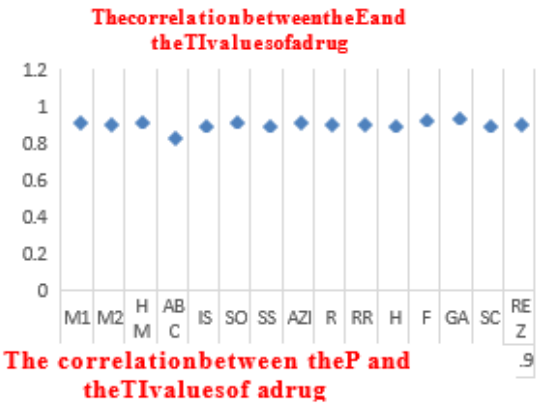


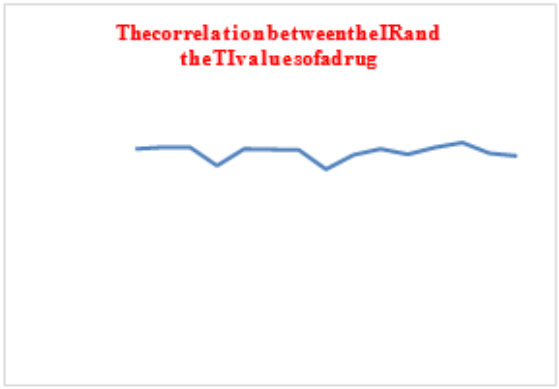




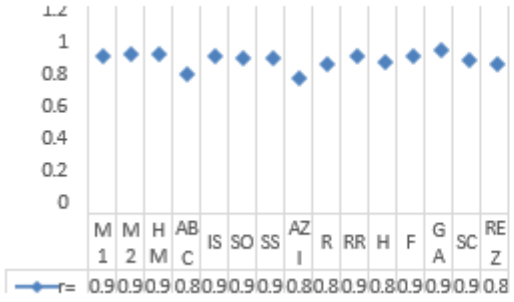


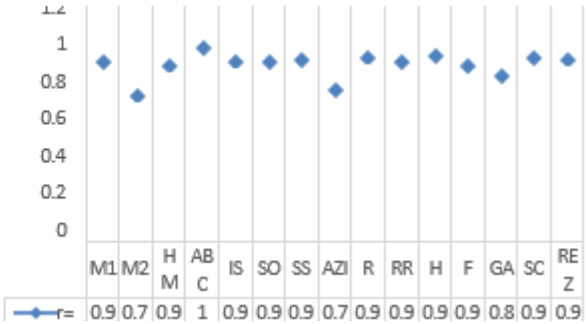


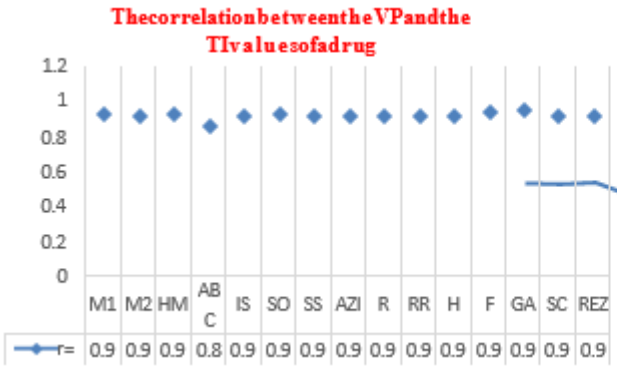


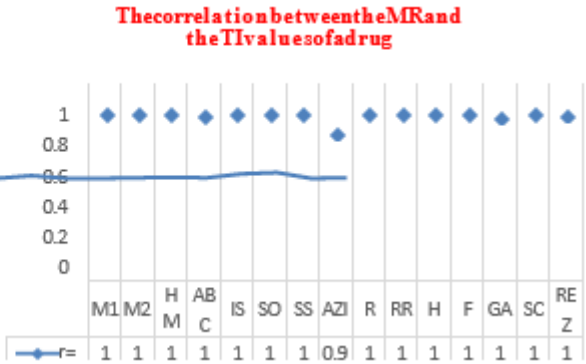


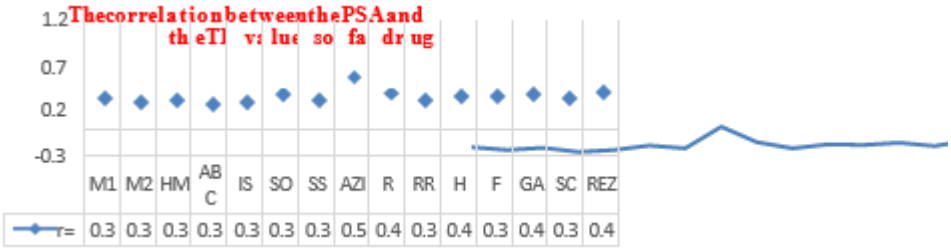
The correlationbetween theP and theTIvaluesof adrug











Conclusion:

Insummary,thisworkaimstousetopologicalindicestopredictimportantphysicochemicalproperties of drugs used in hyper tension treatment. The correlation coefficients in Table 14 would provide insights into how effectivethesetopologicalindicesareforpredictingtheseproperties,whichiscrucialfordevelopingnoveldrugswith desired characteristics efficiently and economically. Overall, the strong correlations observed between Molar Refractionand the topological indices underscore its utility as a keydescriptor inQSPR modeling for predicting and understanding the physicochemicalproperties ofdrugs used in hyper tensiontreatment. This insight can guide future research effortsinoptimizingdrugstructurestoenhancedesiredpropertiesefficientlycorrelateshighlywithM1(H) ,M2(H),HM(H),ABC(H),R(H),RR(H),SS(H),SO(H),ISI(H),H(H),F(H),GA(H),SC(H),RE(H)withan impressivecorrelationcoefficient(r=0.99)andrsquared(r2=0.9).

References:

1.I.Gutman,B.Ruscic,N.Trinajstic,andC.F.WilcoxJr.,“Graphtheoryandmolecularorbitals.XII.Acyclic polyenes,” The Journal of Chemical Physics, vol.62, no.9, pp.3399–3405, 1975.

2.E.Estrada,L.Torres,L.Rodriguez,andI.Gutman,“Anatombondconnectivityindex:modellingtheenthal pyof formation of alkanes,”Indian Journal of Chemistry,vol.37,pp.849–855, 1998.

3. D. Vukicevic and M. Gasperov, “Bond aditive mdelling 1. Ariaticindices,” Croatica Chemica Acta,vol.83,pp.243– 260, 2010.

4. W.Zhao,M.C.Shanmukha,A.Usha,M.R.Farahani,andK.C.Shilpa,“computingSSindexofcertain dendrimers,” Journal of Mathematics, vol. 2021, Article ID 7483508, 14 pages, 2021.

5. M.Randic,“Characterizationofmolecular branching,” Journal oftheAmericanChemical Society,vol.97,no.23,
pp. 6609–6615, 1975.

6. I.Gutman,B.Furtula,andC.Elphick,“Threenew/oldvertex–degree basedtopologicalindices,”MATCHCommunications Mathematical and in Computer Chemistry, vol. 72, pp. 617–632, 2014.

7. S.Fajtlowicz,“OnconjecturesofgrafittiII,”CongressusNumerantium, vol.60,pp.189–197,1987.

8. B. Furtula and I. Gutman, “Aforgotton topological index,” Journal of Mathematical Chemistry, vol.53, pp.213–220,2015.

9. M.Imran, M. Naeem, and A.Q. Baig,“Topological indices of polyhydroxy but rate and polycaprolactone,” Journal of Information and Optimization Sciences, vol. 41, no. 4, pp. 1025–1041, 2020.

10.VukicevicD.,FurtulaB.,Topologicalindexbasedontheratiosofgeometricalandarithmeticalmeansofend-vertex degrees of edges, J. Math. Chem. 2009, 46, 1369-1376.