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Harnessing Topological Indices in QSPR: Predicting Molecular Properties for Parkinson's Disease Therapeutics

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ABSTRACT: Topological indices are numerical invariants derived from molecular graphs play a crucial role in Quantitative Structure-Property Relationship (QSPR) modeling, helping in the prediction of molecular properties relevant to drug discovery. In this study, we predicted eight physicochemical characteristics (PC-C) of thirteen Parkinson's illness medicines through QSPR analysis and topological indices. We computed these indices using Python-based tools (RDKit, NetworkX) and performed regression analysis using Scikit-learn and SciPy. The results show that how some topological indices exhibit strong correlations with several PC-C, demonstrating their value in drug development pipelines.

Keywords: QSPR, SMILES, Parkinson's disease.

Contents

1. Introduction

Molecular property predictions are a cornerstone of modern chemistry and are pertinent to a wide variety of applications from drug design to materials science. Traditional experimental methods for the prediction of such properties are typically time and resource-intensive. Therefore, computational methods that provide rapid and reproducible predictions have been in the limelight of the recent past. Among these, QSPR research has particular importance, since it leverages the intrinsic relationship among the arrangement of a molecule and its PC-C. Topological indices (TI) are quantitative parameters obtained from molecular graphs of Parkinson's disease drugs are an extremely efficient and computer-friendly way of encoding structural information. The TI transfer important properties such as branching, connectivity, and molecular size, and have already demonstrated a tremendous potential for the prediction of a very broad variety of molecular properties. However, the performance of a given topological index can also be capricious concerning the properties under consideration. Their predictability must therefore be investigated systematically, particularly with complicated biological systems.

Parkinson's disease (PD) is a persistent neurological problem that mostly influences motor function. Pathophysiology of PD involves a heterogeneous spectrum of motor and non-motor manifestations and therefore molecular property characterization of drug candidates is necessary. Physical properties such as lipophilicity, polarizability, and electronic properties determine their safety and efficacy. TI and other molecular descriptors can be used in QSPR studies which can be of great help in this regard by offering the facilities of rapid screening and lead prioritization of compounds with desired characteristics. In this work, we implemented Python-based computational techniques using Python libraries such as RDKit (for TI calculations), NetworkX (for graph-based topological index computation using SMILES), and Scikit-learn/SciPy (for correlation and regression analysis). and optimization of the potential candidates in the treatment of PD. This research seeks to determine whether particular graph-theoretical topological indices can quantitatively predict the chemical characteristics of pharmaceuticals used in the therapy of PD via Python-based techniques [1]- [4].

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2. Methods and Methodology

This work used QSPR modeling to examine the relationship among molecular structure and chemical activity about certain aspects relevant to PD medication development. We employed a data set of molecular representations of promising therapeutic candidates with a special focus on TI.

- Data Preparation: Molecular compounds were represented as molecular graphs. TI M1, M2, RA, ABC, SC, GA, H, HZ, and F were calculated for each drug of PDusing SMILES from the Python library RDKit and NetworkX. SMILES were derived from Pubchem (National Library of Medicine). The indices are, each describing different information on the structural properties of the molecules.

- Construction of Models: We design linear regression frameworks utilizing the TI as independent factors and the physical characteristics as follows: i) Boiling point (BP), ii) Enthalpy of vapourization (EV), iii) Flash Point (FP), iv) Molar refractivity (MR), v) Polar surface area (PSA), vi) Polarization (PO), vii) Surface tension(ST), and viii) Molar volume (MV) as dependent variables using Python libraries Scikit-learn and Statsmodels libraries.

- Statistical Analysis: The model performance was validated by employing various measures such as the coefficient of determination (R^2), correlation coefficient (R), p-values (P), and F-statistic (F). The measures provided feedback on the precision and significance of the prediction model using Python libraries Scikit-learn and Statsmodels libraries.

- Interpretation: The findings were interpreted to identify which of the TI contributed most to the molecular properties and biological activity. Interpretation will facilitate the forecasting of patterns applicable in the advancement of novel pharmacological therapies for PD. With the help of computational modeling techniques and topological descriptors, the process is most likely to drive drug discovery ahead in an optimized manner, thereby creating improved therapeutic interventions against Parkinson's disease.

Definition 2.1 *Let be a graph with set of vertices $V(G)$ and set of edges $V(G)$. The term $d(u)$ denotes the degree of the vertex, and it represents the number of edges incident on vertex u.*

Definition 2.2 *The ABC index of a graph G is defined as [5]*

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

Definition 2.3 *The Randić index of a graph G is defined as [6], [7]*

$$RA(G) = \sum_{uv \in E(G)} \frac{1}{2\sqrt{d(u)d(v)}}$$

Definition 2.4 *The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as [8]*

$$M_1(G) = \sum_{uv \in E(G)} d(u) + d(v)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u) \times d(v)$$

Definition 2.5 *The Harmonic index $H(G)$ is defined as [9]:*

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$$

Definition 2.6 *The sum connectivity index $\chi(G)$ is defined as [10],*

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}$$

Definition 2.7 *The Forgotten index of a graph G is defined as [11]:*

$$F(G) = \sum_{uv \in E(G)} (d(u))^2 + (d(v))^2$$

Definition 2.8 *The GA index of a graph G is defined as [12]*

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

Definition 2.9 *The Hyper Zagreb index $HM(G)$ is defined as [13],*

$$HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2$$

3. Results and Discussions

The linear regression approach $Y = a + b(TI)$ relates certain physical characteristics (Y) of thirteen Parkinson's disorder medications with nine TI (See Table 1, where a and b are constants. The following linear regression models are derived (see Table 2).

Table 1: Topological indices of various drugs used in Parkinson's disease.

Molecule	M_1	M_2	R	ABC	SC	GA	H	HM	F
Dopamine	50	55	5.2364	7.9565	5.2217	10.5738	5.0000	326	124
Amantadine	68	82	5.2349	9.3513	5.6969	12.4466	5.0000	596	194
Benzatropine	124	147	11.3097	18.3324	11.9996	25.6236	11.1333	808	310
Trihexyphenidyl	112	130	10.7886	17.0063	11.2419	23.5809	10.6048	772	282
Safinamide	106	117	10.5417	16.6606	10.7748	22.2217	10.1333	682	262
Rasagiline	64	74	6.4150	9.8186	6.6299	13.8418	6.3333	388	154
Entacapone	104	120	10.3490	15.9011	10.2982	20.9767	9.7667	752	272
Opicapone	146	178	12.6288	21.0458	13.0684	27.6326	11.8667	1142	400
Tolcapone	102	119	9.3968	15.3034	9.6190	20.0345	8.8667	750	270
Selegiline	62	67	6.7364	10.0778	6.7217	13.5738	6.5000	374	148
Levodopa	66	73	6.5029	10.3656	6.4998	13.2089	6.0667	474	172
Apomorphine	116	145	9.6647	16.2681	10.3437	22.4364	9.3667	860	310
Rotigotine	112	130	10.7752	16.9586	11.2214	23.5866	10.5667	712	276

Table 2: Regression models.

Model	**Regression Equations**
Regression model of M_1	
	BP = 195.6069 + 2.2844 * M_1
	MR = 14.1167 + 0.6120 * M_1
	EV = 42.3594 + 0.2780 * M_1
	PSA = 18.1934 + 0.4611 * M_1
	FP = 85.7693 + 1.1528 * M_1

	PO = 5.5863 + 0.2428 * M_1 ST = 49.1997 + 0.0656 * M_1 MV = -145.1117 + 5.8354 * M_1
Regression model of M_2	
	BP = 222.1529 + 1.7184 * M_2 MR = 20.4819 + 0.4671 * M_2 EV = 45.4497 + 0.2104 * M_2 PSA = 22.7897 + 0.3554 * M_2 FP = 97.5265 + 0.8820 * M_2 PO = 8.1086 + 0.1853 * M_2 ST = 49.0709 + 0.0574 * M_2 MV = -53.8376 + 4.1772 * M_2
Regression model of RA	
	BP = 153.5778 + 29.0773 * RA MR = 5.3080 + 7.5142 * RA EV = 37.5361 + 3.5060 * RA PSA = 13.9238 + 5.3279 * RA FP = 66.8112 + 14.4207 * RA PO = 2.0909 + 2.9808 * RA ST = 50.7446 + 0.5254 * RA MV = -343.8705 + 84.5564 * RA
Regression model of ABC	
	BP = 169.3919 + 17.0508 * ABC MR = 8.6131 + 4.4612 * ABC EV = 39.3338 + 2.0636 * ABC PSA = 14.1606 + 3.3300 * ABC FP = 74.2046 + 8.4878 * ABC PO = 3.4049 + 1.7695 * ABC ST = 49.5942 + 0.4090 * ABC MV = -247.9973 + 46.0789 * ABC
Regression model of SC	
	BP = 168.7048 + 26.5141 * SC MR = 6.3706 + 7.1619 * SC EV = 39.4257 + 3.1898 * SC PSA = 24.8276 + 4.0220 * SC FP = 75.8402 + 12.9831 * SC PO = 2.5135 + 2.8409 * SC ST = 52.2813 + 0.3414 * SC MV = -346.7278 + 82.2057 * SC
Regression model of GA	
	BP = 183.5218 + 11.8984 * GA MR = 8.4785 + 3.3125 * GA EV = 41.2196 + 1.4309 * GA PSA = 31.0804 + 1.6100 * GA FP = 83.6717 + 5.7963 * GA PO = 3.3499 + 1.3140 * GA ST = 52.9701 + 0.1273 * GA MV = -315.9261 + 37.6784 * GA
Regression model of H	
	BP = 162.8273 + 29.1400 * H

	MR = 4.8706 + 7.8609 * H
	EV = 38.8013 + 3.4961 * H
	PSA = 27.5105 + 4.0005 * H
	FP = 73.6213 + 14.1919 * H
	PO = 1.9173 + 3.1183 * H
	ST = 53.3527 + 0.2411 * H
	MV = -410.5157 + 95.6738 * H
Regression model of HM	
	BP = 235.3829 + 0.2660 * HM
	MR = 27.5781 + 0.0670 * HM
	EV = 46.5845 + 0.0333 * HM
	PSA = 5.3672 + 0.0859 * HM
	FP = 99.4754 + 0.1438 * HM
	PO = 10.9251 + 0.0266 * HM
	ST = 44.8743 + 0.0159 * HM
	MV = 13.1488 + 0.5942 * HM
Regression model of F	
	BP = 213.8507 + 0.8120 * F
	MR = 20.9092 + 0.2097 * F
	EV = 44.2572 + 0.1001 * F
	PSA = 9.8480 + 0.2137 * F
	FP = 91.3303 + 0.4247 * F
	PO = 8.2800 + 0.0832 * F
	ST = 46.4190 + 0.0368 * F
	MV = -25.6775 + 1.7759 * F

Table 3: Physicochemical characteristics and parameters of Parkinson's disease therapeutics.

Molecule	**BP (°C)**	**EV (kJ/mol)**	**FP (°C)**	**MR (cm^3)**	**PSA ($Å^2$)**	**PO (cm^3)**	**ST (d/cm)**	**MV (cm^3)**
Dopamine	337.7	60.4	158.0	43.1	66	17.1	60.8	122.8
Amantadine	225.7	46.2	96.0	45.7	26	18.1	46.8	141.8
Benzatropine	409.0	66.1	120.1	94.6	12	37.5	46.5	274.8
Trihexyphenidyl	447.9	74.4	211.0	91.8	23	36.4	43.3	289.7
Safinamide	476.7	74.0	242.1	83.3	64	33.0	45.1	254.2
Rasagiline	305.5	54.6	146.8	53.9	12	21.4	43.7	162.7
Entacapone	526.6	83.1	272.3	79.1	130	31.4	68.2	219.2
Opicapone	478.2	78.2	243.0	92.5	142	36.7	71.7	229.3
Tolcapone	485.6	78.0	205.7	71.2	103	28.2	66.6	192.5
Selegiline	272.5	51.1	108.4	60.5	3	24.0	37.3	196.2
Levodopa	448.4	74.5	225.0	49.3	104	19.5	80.2	134.3
Apomorphine	473.4	76.5	268.8	77.9	44	30.9	58.3	205.6
Rotigotine	470.1	76.1	238.1	94.6	52	37.5	51.9	272.4

Table 4: Statistical Measures for BP.

Index	**N**	**a**	**b**	**R**	**R^2**	**P**	**F**
M_1	13	195.61	2.28	0.7077	0.5008	0.0068	11.04

Index	N	a	b	R	R^2	P	F
M_2	13	222.15	1.72	0.6733	0.4533	0.0117	9.12
RA	13	153.58	29.08	0.7711	0.5945	0.0020	16.13
ABC	13	169.39	17.05	0.7472	0.5583	0.0033	13.90
SC	13	168.70	26.51	0.7413	0.5495	0.0037	13.42
GA	13	183.52	11.90	0.7158	0.5123	0.0059	11.56
H	13	162.83	29.14	0.7485	0.5603	0.0032	14.02
HM	13	235.38	0.27	0.6439	0.4146	0.0175	7.79
F	13	213.85	0.81	0.6845	0.4686	0.0098	9.70

Table 4 shows that RA index is the good predictor for boiling point with R^2 value of 0.5945. The model is statistically significant with a p-value of 0.0020.

Table 5: Statistical Measures for EV.

Index	N	A	b	R	R^2	P	F
M_1	13	42.36	0.28	0.6894	0.4753	0.0091	9.96
M_2	13	45.45	0.21	0.6599	0.4354	0.0141	8.48
RA	13	37.54	3.51	0.7442	0.5538	0.0035	13.65
ABC	13	39.33	2.06	0.7238	0.5239	0.0052	12.10
SC	13	39.43	3.19	0.7138	0.5095	0.0061	11.43
GA	13	41.22	1.43	0.6890	0.4747	0.0092	9.94
H	13	38.80	3.50	0.7188	0.5167	0.0056	11.76
HM	13	46.58	0.03	0.6452	0.4163	0.0172	7.85
F	13	44.26	0.10	0.6758	0.4567	0.0112	9.25

Table 5 shows that RA index is the good predictor for EV with R^2 value of 0.5538.

Table 6: Statistical Measures for FP.

Index	N	A	b	R	R^2	P	F
M_1	13	85.77	1.15	0.5489	0.3013	0.0520	4.74
M_2	13	97.53	0.88	0.5312	0.2822	0.0618	4.32
RA	13	66.81	14.42	0.5878	0.3455	0.0346	5.81
ABC	13	74.20	8.49	0.5717	0.3269	0.0412	5.34
SC	13	75.84	12.98	0.5579	0.3113	0.0475	4.97
GA	13	83.67	5.80	0.5360	0.2873	0.0590	4.43
H	13	73.62	14.19	0.5604	0.3140	0.0464	5.04
HM	13	99.48	0.14	0.5352	0.2864	0.0595	4.41
F	13	91.33	0.42	0.5504	0.3029	0.0513	4.78

Table 6 shows that RA index is the good predictor for FP.

Table 7: Statistical Measures for MR.

Index	N	A	b	R	R^2	P	F
M_1	13	14.12	0.61	0.9234	0.8526	6.71E-06	63.65
M_2	13	20.48	0.47	0.8914	0.7946	4.29E-05	42.55
RA	13	5.31	7.51	0.9705	0.9419	3.87E-08	178.17
ABC	13	8.61	4.46	0.9521	0.9066	5.33E-07	106.75

Index	N	A	b	R	R^2	P	F
SC	13	6.37	7.16	0.9752	0.9511	1.49E-08	213.75
GA	13	8.48	3.31	0.9706	0.9420	3.81E-08	178.68
H	13	4.87	7.86	0.9835	0.9673	1.63E-09	324.90
HM	13	27.58	0.07	0.7904	0.6247	0.0013	18.31
F	13	20.91	0.21	0.8612	0.7416	0.0002	31.57

Table 7 shows that H index is the good predictotr for MR among other indices with R^2 value of 0.9673.

Table 8: Statistical Measures for PSA.

Index	N	a	b	R	R^2	P	F
M_1	12	18.19	0.46	0.2860	0.0818	0.3676	0.89
M_2	12	22.79	0.36	0.2820	0.0795	0.3745	0.86
RA	12	13.92	5.33	0.2646	0.0700	0.4060	0.75
ABC	12	14.16	3.33	0.2842	0.0808	0.3707	0.88
SC	12	24.83	4.02	0.2151	0.0463	0.5020	0.48
GA	12	31.08	1.61	0.1884	0.0355	0.5577	0.37
H	12	27.51	4.00	0.1923	0.0370	0.5494	0.38
HM	12	5.37	0.09	0.4311	0.1858	0.1618	2.28
F	12	9.85	0.21	0.3683	0.1356	0.2388	1.57

Table 8 shows that HM index is the best predictor for PSA with R^2 value of 0.1858.

Table 9: Statistical Measures for PO.

Index	N	a	b	R	R^2	P	F
M_1	13	14.12	0.61	0.9234	0.8526	6.71E-06	63.65
M_2	13	20.48	0.47	0.8914	0.7946	4.29E-05	42.55
RA	13	5.31	7.51	0.9705	0.9419	3.87E-08	178.17
ABC	13	8.61	4.46	0.9521	0.9066	5.33E-07	106.75
SC	13	6.37	7.16	0.9752	0.9511	1.49E-08	213.75
GA	13	8.48	3.31	0.9706	0.9420	3.81E-08	178.68
H	13	4.87	7.86	0.9835	0.9673	1.63E-09	324.90
HM	13	27.58	0.07	0.7904	0.6247	0.0013	18.31
F	13	20.91	0.21	0.8612	0.7416	0.0002	31.57

Table 9 shows that H index is the best predictor for PO with R^2 value of 0.9673.

Table 10: Statistical Measures for ST.

Index	N	a	b	R	R^2	P	F
M_1	13	49.20	0.07	0.1460	0.0213	0.6341	0.24
M_2	13	49.07	0.06	0.1616	0.0261	0.5979	0.29
RA	13	50.74	0.53	0.1001	0.0100	0.7449	0.11
ABC	13	49.59	0.41	0.1288	0.0166	0.6750	0.19
SC	13	52.28	0.34	0.0686	0.0047	0.8238	0.05
GA	13	52.97	0.13	0.0550	0.0030	0.8583	0.03
H	13	53.35	0.24	0.0445	0.0020	0.8852	0.02
HM	13	44.87	0.02	0.2760	0.0762	0.3614	0.91
F	13	46.42	0.04	0.2232	0.0498	0.4635	0.58

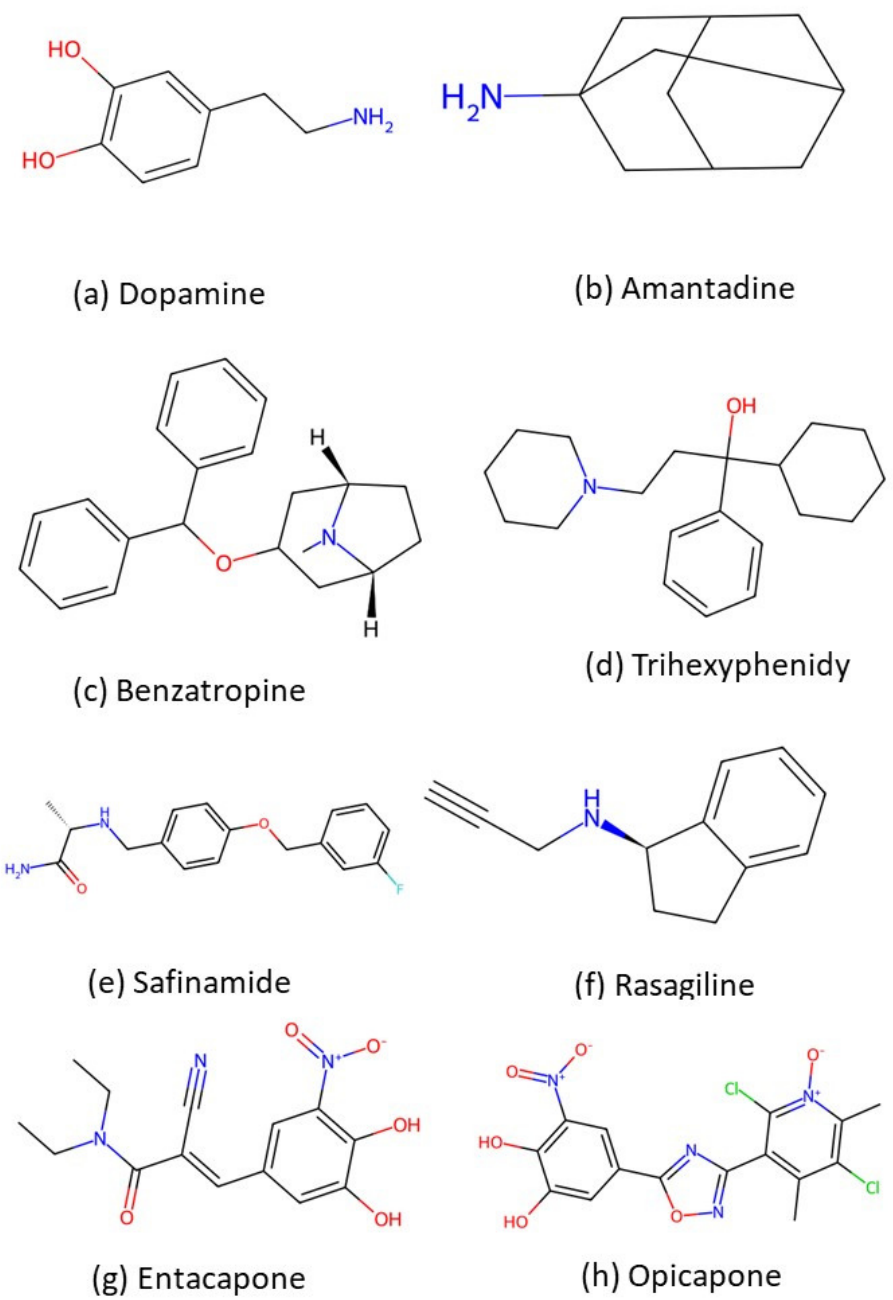

Figure 1: Molecular structures of Parkinson's disease drugs (a) Dopamine (b) Amantadine (c) Benzatropine (d) Trihexyphenidy (e) Safinamide (f) Rasagiline (g) Entacapone (h) Opicapone.

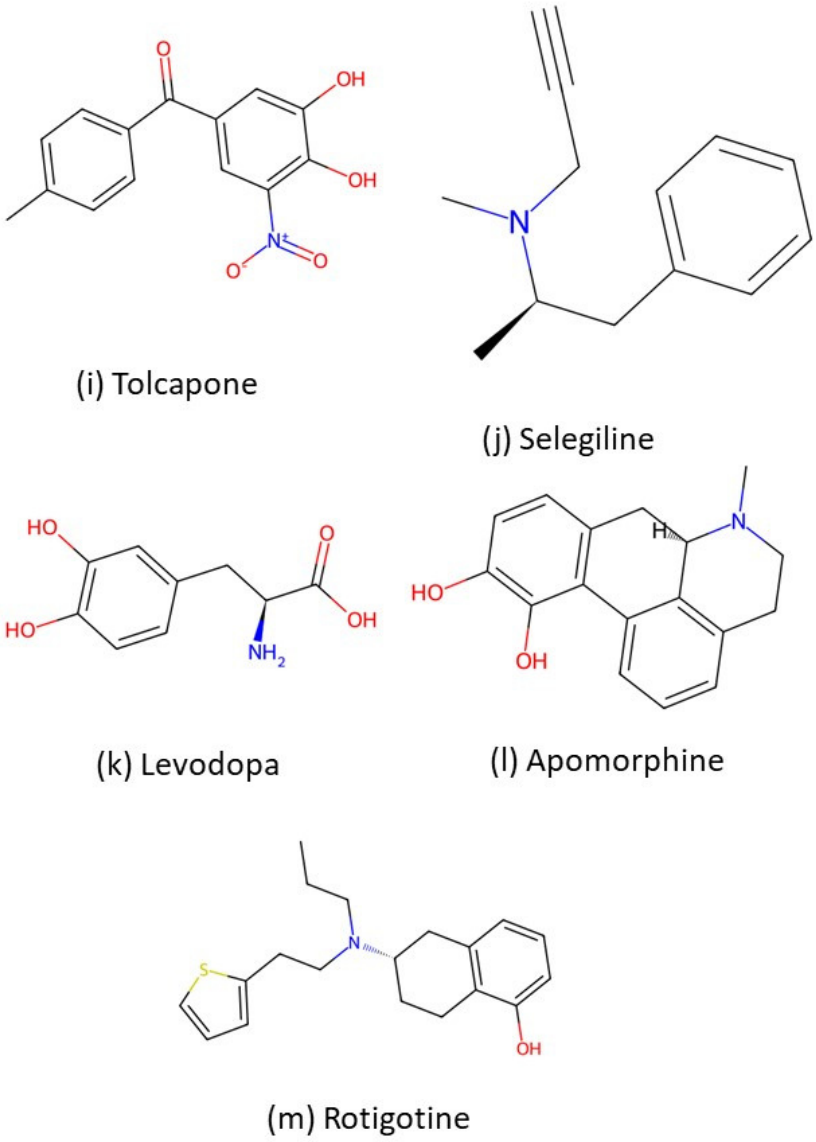

Figure 2: Molecular structures of Parkinson's disease drugs (i) Tolcapone (j) Selegilibe (k) Levodopa (l) Apomorphine (m) Rotigotine.

Table 10 shows that HM index is the best predictor for ST with R^2 value of 0.0762.

Table 11: Statistical Measures for MV.

Index	N	a	b	R	R^2	P	F
M_1	13	-145.11	5.84	0.2287	0.0523	0.4523	0.61
M_2	13	-53.84	4.18	0.2071	0.0429	0.4973	0.49
RA	13	-343.87	84.56	0.2837	0.0805	0.3476	1.00
ABC	13	-248.00	46.08	0.2555	0.0653	0.3996	0.77
SC	13	-346.73	82.21	0.2908	0.0845	0.3351	1.02
GA	13	-315.93	37.68	0.2868	0.0822	0.3421	0.99
H	13	-410.52	95.67	0.3109	0.0967	0.3011	1.18
HM	13	13.15	0.59	0.1820	0.0331	0.5518	0.38
F	13	-25.68	1.78	0.1894	0.0359	0.5354	0.41

Table 11 shows that HM index is the good predictor for MV with the R^2 value of 0.0331. From these results, it is clear that, although the above molecular properties are important in the design of drugs, it might require other molecular descriptors or properties to provide improved predictive accuracy in QSPR modeling. Figure 3 shows a positive regression correlation between BP and RA index. RA becomes the

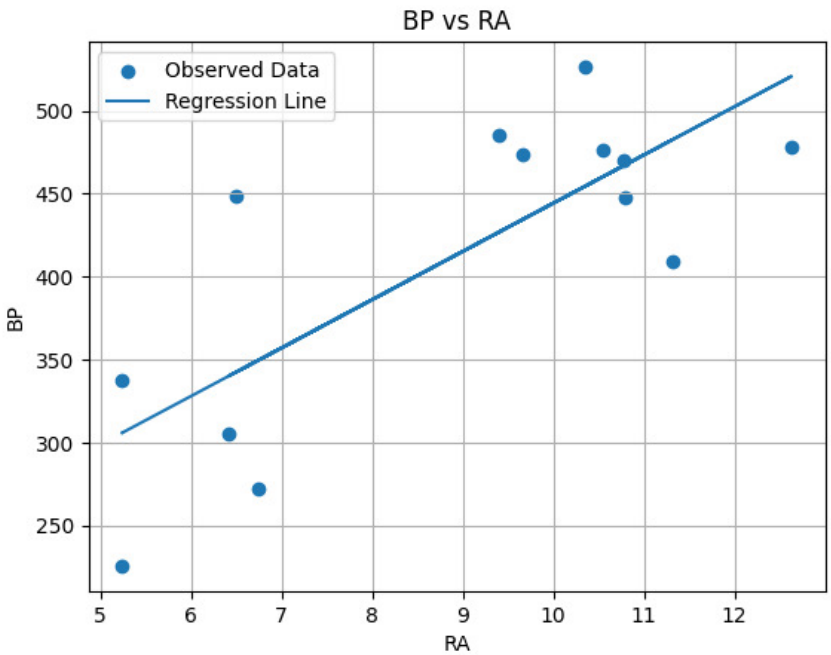

Figure 3: Linear regression graphs between BP and RA.

best predictive index for BP. It suggests that molecular topology (connectivity) significantly influences a physical property (boiling point).

Figure 4 shows that as RA increases, the enthalpy of vaporization (EV) also increases. This implies that more structurally complex or branched molecules tend to require more energy to vaporize. EV is an important parameter for formulation, drug delivery, storage, and safety. Figure 2.4 indicates that RA alone may not be sufficient for predicting EV. Additional TI may be required [14,15,16,17].

Figure 5 shows a positive correlation between H Index and FP. As H increases, FP increases indicate that molecules with more branched or complex connectivity tend to have higher flash points. The flash

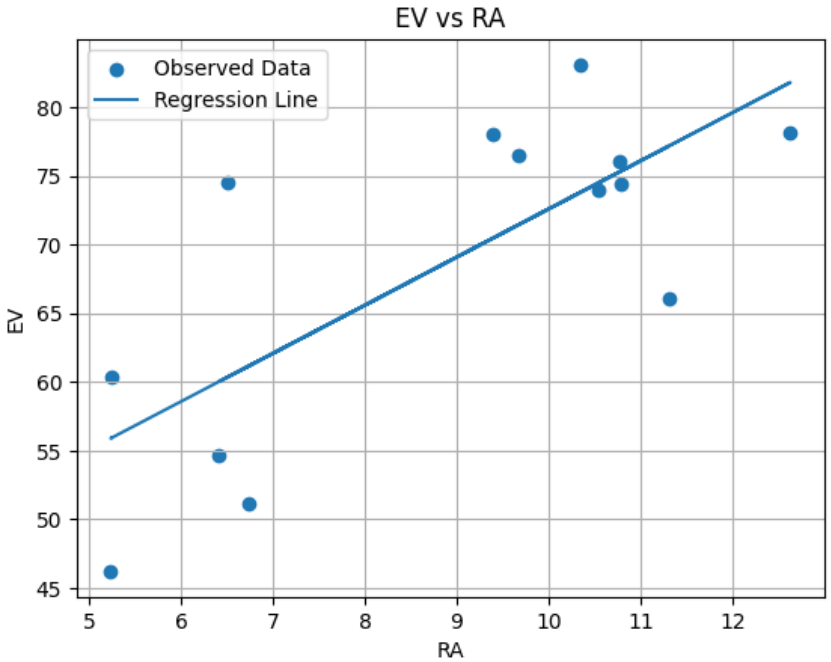

Figure 4: Linear regression graphs between EV and RA.

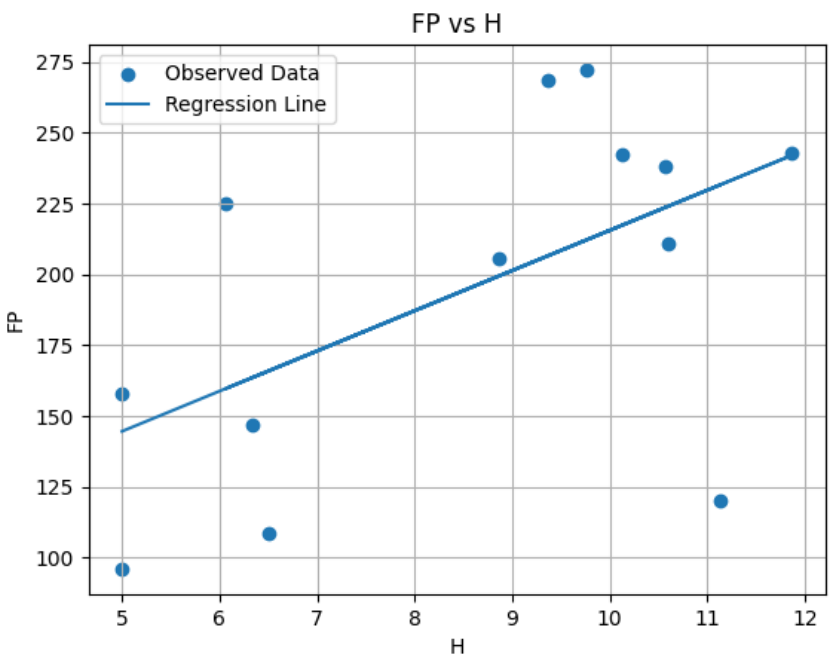

Figure 5: Linear regression graphs between FP and H.

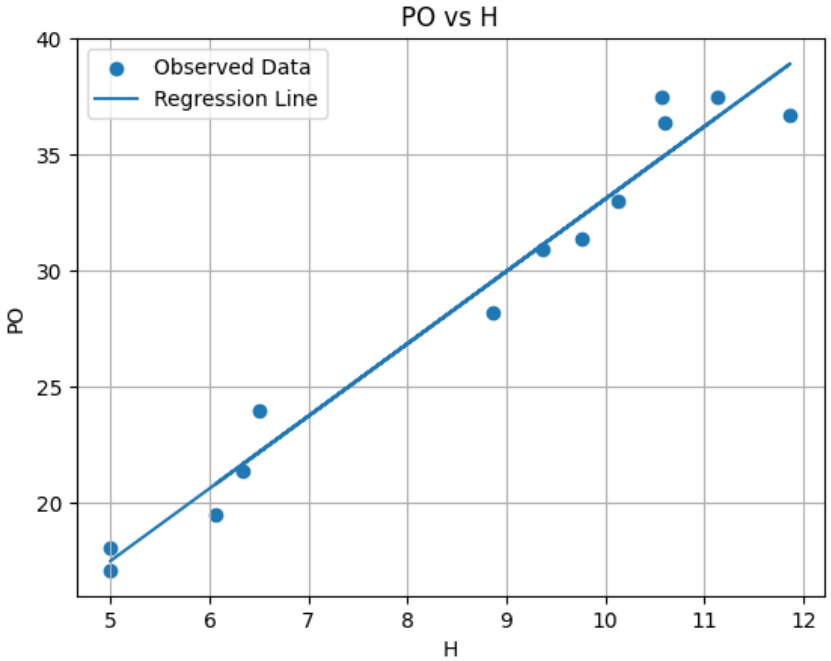

Figure 6: Linear regression graphs between PO and H.

point is important for Storage and transport decisions, formulation safety and material handling protocols.

Figure 6 shows a strong positive correlation between PO and H. A higher H index reflects greater polarizability, meaning these molecules respond more easily to electric fields, which is crucial for drug-receptor interactions.

4. Conclusion

This study demonstrates the features of quantitative structure-property relationship (QSPR) modeling with the utility of discovering the relationship between molecular properties and biological activities needed to develop drugs to treat Parkinson's disease. The study employs TI as potential descriptors and shows that RA and M1 indices are promising predictors of different molecular properties related to biological activity, molecular refractivity, and electrostatic potential. In essence, RA emerged as the main predictor, with the highest values obtained across some of the molecular properties. The RA index clearly showed a strong association with molecular refractivity, suggesting that size and shape are important properties for drug effectiveness, while the models predicting hydrophobicity and solubility properties were less predictable but still informative. The low predictability for some of the properties shows the complexity involved in prediction and the likely need for additional molecular descriptors. The study also indicated the difficulty of predicting other important properties like solubility and molecular volume, which failed to define a solid modeling strategy. This suggests the necessity to enhance QSPR modeling and explore other computational algorithms to further enhance the prediction of hyper- PC-C, which are of very critical significance in drug design. To facilitate the calculation and statistical analysis of TI, the study heavily relied on Python-based libraries, such as RDKit for the computation of TI, NetworkX for the graphical representation of molecular structures, Pandas for data manipulation, and Scikit-learn for regression modeling and predictive processing. The integration of these computational tools allowed for the methodical assessment of molecular characteristics, reinforcing the applicability of machine learning techniques in QSPR research.

The use of these computational libraries enabled the systematic analysis of molecular properties, which warrants the use of machine learning techniques in QSPR studies. Lastly, this study confirms the use of

TI in QSPR studies and facilitates further study to enhance pharmacological treatments for Parkinson's illness. The findings of this advance the science of computational drug design and propose directions for future studies. Additional studies in this field will be critical to advance our knowledge of molecular interactions in neurological diseases and to optimize therapeutics for neurological diseases.

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