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QSPR ANALYSIS AND DEGREE-BASED MOLECULAR DESCRIPTIONS OF RENAL THERAPY DRUGS

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Abstract:
This study determines the quantitative structure-property relationship (QSPR) of five renal therapy Medicines in this article. QSPR is a computational chemistry approach that correlates a compound's molecular structure with its physical, chemical, and biological characteristics. In this situation, the features of interest are most likely linked to the effectiveness or pharmacological behaviours of the therapeutic medications.

Keywords: QSPR, Topological Indices, Molecular structures, and renal therapy.
Subject Classification: 05C92

Introduction:

Kidney is the best multi-tasking on your body's backstage crew. This bean-shaped organ is part of the urinary System and serves as the body's final filter, cleaning blood by eliminating waste and excess fluids before producing urine. It also has an unanticipated effect on blood pressure regulation, electrolyte balance, and even red blood cell synthesis. In short, the kidney is an unsung hero who silently does its ultimate function behind the scenes. Several risk factors can contribute to kidney problems or diseases. Some common risk factors include:

Diabetes: High blood sugar levels can damage the kidneys over time.
High blood pressure: Hypertension can strain the blood vessels in the kidneys, leading to kidney damage.
Family history: A family history of kidney disease can increase your risk.
Age: The risk of kidney disease increases with age.
Obesity: Being overweight or obese can increase the risk of developing kidney disease.
Smoking: Smoking can damage blood vessels, including those in the kidneys.
Heart disease: Conditions that affect the heart can also impact kidney function.
Certain medications: Some medications can harm the kidneys, especially when taken over a long period.
High cholesterol: Elevated cholesterol levels can contribute to kidney problems.
Race or ethnicity: Certain ethnic groups, such as African Americans, Hispanics, and Native Americans, have a higher risk of developing kidney disease.

Managing these risk factors through lifestyle changes, regular health check-ups, and medication management can help reduce the likelihood of kidney problems.

1.Non-Modifiable Risk Factors

Non-modifiable risk factors for kidney disease are those that cannot be changed or controlled. These factors include:

1. **Age**: The risk of kidney disease generally increases with age, especially after 65 years.
2. **Genetics/Family History**: A family history of kidney disease can increase your risk. Certain genetic factors May predispose individuals to kidney problems.

3. Race/Ethnicity: Some ethnic groups, such as African Americans, Hispanics, Native Americans, and Pacific Islanders, have a higher risk of developing certain types of kidney disease compared to others.

These non-modifiable risk factors underscore the importance of regular health screenings and awareness, particularly for individuals with a family history of kidney disease or those belonging to high-risk ethnic groups. While these factors cannot be changed, early detection and management can help mitigate risks and improve outcomes.Kidney disease can be broadly categorized into several types based on different criteria. Here are some common categories of kidney disease:

1. **Acute Kidney Injury (AKI)**: This refers to a sudden loss of kidney function, often due to conditions like Dehydration, severe infection, or medication toxicity.
2. **Chronic Kidney Disease (CKD)**: This is a long-term condition where kidneys gradually lose their function over time, usually caused by conditions like diabetes, high blood pressure, or autoimmune diseases.
3. **Glomerular Diseases**: These affect the glomeruli, the tiny filters in the kidneys. Examples include glomerulonephritis, which can be acute or chronic.
4. **Polycystic Kidney Disease (PKD)**: This is an inherited disorder where clusters of cysts develop within the kidneys, eventually leading to kidney failure.
5. **Kidney Stones**: These are solid crystals that form in the kidneys and can cause severe pain and obstruction of the urinary tract.
6. **Urinary Tract Infections (UTIs)**: While not always directly a kidney disease, recurrent or severe UTIs can lead to kidney damage if left untreated.
7. **Nephrotic Syndrome**: A group of symptoms that indicate kidney damage, including protein in the urine, low blood protein levels, high cholesterol levels, and swelling.
8. **Congenital Kidney Disorders**: These are kidney problems that are present at birth, such as abnormalities in kidney structure or function.
9. **Diabetic Nephropathy**: Kidney damage caused by diabetes, which is a common cause of chronic kidney disease.

Each category may have various subtypes and degrees of severity, and treatment approaches vary depending on the specific condition and its stage.\

2. Topological index significance and Applications:

Topological indices are numerical values associated with the structure of a molecule, derived from its graph-theoretical properties. These indices play a crucial role in the study of chemical graph theory and molecular chemistry. They provide insights into the molecular structure, properties, and behavior, which are essential for various applications in chemistry, pharmacology, and materials science.

Methods:

Several methodologies, including QSAR, QSPR, and QSTR, allow chemists or pharmacists to use drug-related data, such as melting point, boiling point, molar refractivity, density, enthalpy, vaporization, flash point, polar surface 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 various aspects of this ailment. Drug selection for QSPR analysis based on topological indices takes into account both 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 kidney treatment is 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 by V and E, respectively.

Definition:1.1: The first and second Zagreb indices are among the primitive indices designed by Trinajstic and Gutman, which are defined as [1]

$$M1(\mathfrak{G})=\sum e\epsilon E(\mathfrak{G})(\delta a+\delta b),$$

$M2(\mathfrak{G})=\sum e\epsilon E(\mathfrak{G})(\delta a\delta b)$

Definition:1.2: Harmonic Index is given by [7]

$$H(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{2}{\delta_a + \delta_b}$$

Definition:1.3: Randic Index introduced [5]

$$R(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{1}{\sqrt{\delta_a.\delta_b}}$$

Definition:1.4: Estrada Index introduced [2]

$$ABC(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{\sqrt{\delta_a + \delta_b - 2}}{\delta_a.\delta_b}$$

Definition:1.5: Vukicevicet al[3]introduced Inverse Indeg Index as

$$IS(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{\delta_a.\delta_b}{\delta_a + \delta_b}$$

Definition:1.6: Zhaoetal.[4] formulated the SS index which is defined as

$$SS(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{\delta_a.\delta_b}{\sqrt{\delta_a + \delta_b}}$$

Definition:1.7: Gutman formulated the sombor index which is defined as

$$SO(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \sqrt{(\delta_a)^2 + (\delta_b)^2}$$

Definition:1.8: Reciprocal Randic Index introduced [6]

$$RR(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \sqrt{(\delta_a.\delta_b)}$$

Definition:1.9: Hyper Zagreb Index

$$HM(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{2}{\delta_a + \delta_b}$$

Definition:1.10: Augmented Zagreb Index

$$AZI(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} \frac{(\delta_a.\delta_b)^3}{\delta_a + \delta_b - 2}$$

Definition:1.11: Forgetton Index

$$F(\mathfrak{I}) = \sum_{e\in E(\mathfrak{I})} (\delta_a + \delta_b)^3$$

TABLE : PHYSICO CHEMICAL PROPERTIES OF RENAL THERAPY DRUGS

Drug Name	D	BP	VP	E	FP	IR	MR	PSA	P	ST	MV
Captopril	1.3	427	2.2	74.8	212.1	1.55	54.4	96	21.6	54.3	170.7
Finerenpril	1.3	554.7	1.5	83.6	289.3	1.63	103.7	11	63.5	41.1	292.8
Fosinopril	1.2	705.7	2.4	108.4	380.6	1.53	148.8	120	48.4	59	480.4
Lisinopril	1.3	666.4	2.1	102.9	356.9	1.58	107.5	133	60.4	42.6	323.9
Rampril	1.2	616.2	1.9	96.1	326.4	1.57	111.4	96	44.2	50.2	346.8

TABLE : COMPUTED VALUES OF TI's OF RENAL THERAPY DRUGS

Drug Name	M1	M2	ABC	IS	SS	AZI	SO	R	RR	H	F	HM
Captopril	66	76	10.18	11.67	14.46	107.06	48.32	6.6	32.01	6.2	132	324
Finerenpril	137	166	19.98	32.38	29.84	132.63	99.41	12.48	66.54	11.93	363	695
Fosinopril	165	186	25.89	39.33	37.46	273.57	119.3	15.29	80.5	16.18	409	781
Lisinopril	138	157	20.31	33.11	31.22	239	99.46	13.76	67.55	14.06	384	625
Rampril	146	153	29.39	34.62	32.54	267.34	672.28	14.08	71.01	13.57	370	540

TABLE: Statistical Specifications for the Linear Model of ABC(G)

Physical Properties	N	A	b	r	r2	F
D	5	-0.002	1.327	0.364	0.133	0.458
BP	5	11.89	342.6	0.794	0.631	5.132
VP	5	-0.003	2.078	0.58	0.003	0.01
E	5	1.417	63.27	0.747	0.558	3.789
FP	5	7.189	161.13	0.794	0.63	5.116
IR	5	0.005	1.471	0.839	0.703	7.114
MR	5	3.829	24.24	0.83	0.68	6.615
PSA	5	0.885	72.51	0.135	0.018	0.056
P	5	1.08	24.76	0.474	0.225	0.87
ST	5	0.068	47.99	0.065	0.004	0.013
MV	5	12.45	59.78	0.816	0.666	5.984

TABLE: Statistical Specifications for the Linear Model of M1(G)

Physical Properties	N	A	b	r	r2	F
D	5	-0.01	1.375	0.608	0.369	1.755
BP	5	2.632	244.3	0.927	0.859	18.23
VP	5	-0.01	2.092	0.06	0.004	0.01
E	5	0.31	52.67	0.847	0.718	7.63
FP	5	1.621	104.65	0.926	0.858	18.19
IR	5	0.001	1.518	0.786	0.619	4.86
MR	5	0.859	-6.79	0.96	0.93	37.6
PSA	5	0.09	78.58	0.077	0.006	0.02
P	5	0.325	5.19	0.74	0.54	3.6
ST	5	-0.01	51.2	0.06	0.005	0.01
MV	5	0.085	225.4	0.026	0.001	0.002

TABLE:	Statistical Specifications for the Linear Model of M2(G)					
Physical Properties	N	A	b	r	r2	F
D	5	-0.01	1.35	0.48	0.23	0.879
BP	5	2.31	252.6	0.89	0.792	11.46
VP	5	-0.001	2.18	0.135	0.02	0.06
E	5	0.26	54.86	0.789	0.622	4.9
FP	5	1.398	106.6	0.89	0.792	11.45
IR	5	0	1.486	0.375	0.141	0.491
MR	5	0.757	-6.505	0.945	0.892	24.8
PSA	5	-0.04	97.4	0.04	0.001	0.004
P	5	0.324	-0.209	0.819	0.671	6.1
ST	5	-0.028	53.51	0.152	0.023	0.071
MV	5	-0.008	237.7	0.003	0	0

TABLE:	Statistical Specifications for the Linear Model of IS(G)					
Physical Properties	N	A	b	r	r2	F
D	5	-0.002	1.34	0.474	0.225	0.87
BP	5	9.44	308.64	0.927	0.859	18.29
VP	5	-0.003	2.11	0.089	0.008	0.024
E	5	1.08	60.3	0.843	0.711	7.38
FP	5	5.71	140.55	0.927	0.859	18.24
IR	5	0	1.594	0.113	0.012	0.039
MR	5	2.98	15.03	0.95	0.9	27.57
PSA	5	0.308	81.91	0.069	0.005	0.014
P	5	1.19	11.61	0.767	0.588	4.278
ST	5	-0.82	51.93	0.116	0.013	0.041
MV	5	9.362	40.39	0.902	0.813	13.079

TABLE:	Statistical Specifications for the Linear Model of AZI(G)					
Physical Properties	N	A	b	r	r2	F
D	5	-0.001	1.37	0.8	0.64	5.4
BP	5	1.252	340.63	0.89	0.79	11.4
VP	5	0.002	1.67	0.38	0.14	0.51
E	5	0.165	59.75	0.92	0.86	18.12
FP	5	0.757	159.9	0.89	0.79	11.37
IR	5	0	1.57	0.5	0.25	1.014
MR	5	0.354	33.51	0.82	0.66	5.99
PSA	5	0.36	18.04	0.589	0.347	1.59
P	5	0.065	34.41	0.305	0.093	0.307
ST	5	0.027	43.945	0.277	0.077	0.249
MV	5	1.222	75.63	0.85	0.72	7.97

TABLE:	Statistical Specifications for the Linear Model of H(G)					
Physical Properties	N	A	b	r	r2	F
D	5	-0.009	1.368	0.601	0.361	1.696
BP	5	28.41	242.01	0.984	0.968	90.1
VP	5	0	1.89	0.108	0.012	0.035
E	5	3.43	50.74	0.936	0.877	21.29
FP	5	17.18	100.25	0.984	0.968	89.58
IR	5	-0.001	1.53	0.068	0.005	0.014
MR	5	8.61	-1.49	0.97	0.94	43.16
PSA	5	3.36	49.6	0.27	0.071	0.23
P	5	3.049	9.86	0.69	0.48	2.77
ST	5	-0.1	49.56	0.005	0	0
MV	5	27.72	-20.49	0.94	0.88	23.69

TABLE	Correlation coefficient between physico chemical properties and TI's of Renal Therapy Drugs											
	M1(G)	M2(G)	ABC(G)	IS(G)	RR(G)	F(G)	H(G)	HM(G)	S(G)	AZI(G)	SO(G)	R(G)
D	0.608	0.48	0.364	0.474	0.61	0.468	0.601	0.353	0.621	0.8	0.658	0.597
BP	0.927	0.89	0.794	0.927	0.931	0.92	0.984	0.83	0.94	0.89	0.2	0.955
VP	0.06	0.135	0.58	0.089	0.054	0.15	0.108	0.088	0.006	0.38	0.19	0.019
E	0.847	0.789	0.747	0.843	0.85	0.83	0.936	0.72	0.87	0.92	0.2	0.88
FP	0.926	0.89	0.794	0.927	0.93	0.92	0.984	0.83	0.94	0.89	0.205	0.955
IR	0.786	0.375	0.839	0.113	0.091	0.155	0.068	0.327	0.045	0.5	0.232	0.007
MR	0.96	0.945	0.83	0.95	0.96	0.91	0.97	0.91	0.97	0.82	0.2	0.943
PSA	0.077	0.04	0.135	0.069	0.085	0.052	0.27	0.09	0.13	0.589	0.062	0.17
P	0.74	0.819	0.474	0.767	0.74	0.84	0.69	0.81	0.72	0.305	0.035	0.72
ST	0.06	0.152	0.065	0.116	0.067	0.24	0.005	0.117	0.034	0.277	0.047	0.093
MV	0.026	0.003	0.816	0.902	0.92	0.85	0.94	0.85	0.94	0.85	0.212	0.9

3. Regression Models

The line are regression model is given by

$P=\gamma + (TI)$ ---------- (I)

Where P, δ, TI⟶ physical property of drug, constant, regression coefficient, and topological index. Using equation (I), the line is models for the respective topological indices considered in the study are obtained as follows.

First Zagreb index M1 (G):

D = -0.001+1.375 M1(G)
BP = 2.682+244.33 M1(G)
VP = -0.001+2.092 M1(G)
E = 0.31+52.67 M1(G)
FP = 1.621+104.65 M1(G)
IR = 0.001+1.518 M1(G)
MR = 0.8599-6.79 M1(G)
PSA= 0.09+78.58 M1(G)
P = 0.325+5.19 M1(G)
ST = -0.01+51.2 M1(G)
MV =0.085+225.4 M1(G)

Second Zagreb index M2 (G):

D = -0.001+1.35 M2(G)
BP = 2.31+252.6 M2(G)
VP = -0.001+2.18 M2(G)
E = 0.26+54.86 M2(G)
FP = 1.398+106.6 M2(G)
IR = 0.00+1.486 M2(G)
MR = 0.757-6.505 M2(G)
PSA = -0.04-97.4 M2(G)
P = 0.324-0.209 M2(G)
ST = -0.028-53.51 M2(G)
MV = -0.008-237.7 M2(G)

ABC Index ABC (G):

D = -0.002+1.327 ABC(G)
BP = 11.89+342.6 ABC(G)
VP = -0.003+2.078 ABC(G)
E = 1.417+63.216 ABC(G)
FP = 7.189+161.13 ABC(G)
IR = 0.005+1.471 ABC(G)
MR = 3.829+24.24 ABC(G)
PSA = 0.885+72.51 ABC(G)
P = 1.08+24.76 ABC(G)
ST = 0.068+47.99 ABC(G)
MV = 12.45+59.78 ABC(G)

Inverse indeg index IS (G):

D = -0.002+1.34 IS(G)
BP = 9.44+308.64 IS(G)
VP = -0.003+2.11 IS(G)
E = 1.08+60.3 IS(G)
FP = 5.71+140.55 IS(G)
IR = 0.00+1.594 IS(G)
MR = 2.98+15.03 IS(G)
PSA = 0.308+81.91 IS(G)
P = 1.19+11.67 IS(G)
ST = -0.82+51.93 IS(G)
MV = 9.362+40.39 IS(G)

SO Index SO (G):

D = 0.00+0.28 SO(G)
BP = 0.86+576.10 SO(G)
VP = 0.000+2.07 SO(G)
E = 0.011+90.93 SO(G)
FP = 0.052+302.28 SO(G)
IR = 0.00+1.528 SO(G)
MR = 0.026+99.7 SO(G)
PSA = 0.001+88.85 SO(G)
P = -0.02+48.08 SO(G)
ST = 0.001+49.15 SO(G)
MV = 0.09+304.17 SO(G)

SS Index SS (G)

D = -0.004+1.37 SS(G)
BP = 11.89+247.8 SS(G)
VP = 0.00+2.02 SS(G)
E = 1.39+52.54 SS(G)
FP = 7.19+103.81 SS(G)
IR = 0.00+1.51 SS(G)
MR= 3.76-4.38 SS(G)
PSA = 0.79+69.98 SS(G)
P = 1.375+7.61 SS(G)
ST = -0.03+50.30 SS(G)
MV = 11.98-25.82 SS(G)

Augmented zagreb Index AZI (G):

D = -0.001+1.37 AZI(G)

BP = 1.252+340.63 AZI(G)

VP = 0.002+1.67 AZI(G)

E = 0.165+59.75 AZI(G)

FP = 0.757+159.9 AZI(G)

IR = 0.00+1.57 AZI(G)

MR = 0.354+33.51 AZI(G)

PSA = 0.36+18.04 AZI(G)

P = 0.065+34.41 AZI(G)

ST = 0.027+43.95 AZI(G)

MV = 1.222+75.63 AZI(G)

R Index R (G):

D = -0.010+1.378 R (G)

BP = 30.33+216.33 R (G)

VP = -0.002+2.044 R (G)

E = 3.575+48.63 R (G)

FP = 18.33+84.74 R (G)

IR = 0.00+1.52 R (G)

MR = 9.23-9.83 R (G)

PSA = 2.42+61.09 R (G)

P = 3.548+3.43 R (G)

ST = -0.206+52.004 R (G)

MV = 29.27-41.67 R (G)

RR Index RR (G):

D = -0.002+1.374 RR (G)

BP = 5.503+244.46 RR (G)

VP = -0.001+2.084 RR (G)

E = 0.64+52.62 RR (G)

FP = 3.33+101.75 RR (G)

IR = 0.00+1.51 RR (G)

MR = 1.76-6.36 RR (G)

PSA = 0.22+77.22 RR (G)

P = 0.66+5.34 RR (G)

ST = -0.13+51.21 RR (G)

MV = 5.55-29.61 RR (G)

H Index H (G):

D = -0.009+1.368 H (G)

BP = 28.41+242.01 H (G)

VP = 0.000+1.89 H (G)

E = 3.43+50.74 H (G)

FP = 17.18+100.25 H (G)

IR = -0.001+1.53 H (G)

MR = 8.61-1.49 H (G)

PSA = 3.36+49.60 H (G)

P = 3.049+9.86 H (G)

ST = -0.10+49.56 H (G)

MV = 27.72-20.49 H (G)

F Index F (G):

D = 0.00+1.335 F (G)

BP = 0.889+299.35 F (G)

VP = 0.000+2.17 F (G)

E = 0.101+59.59 F (G)

FP = 0.54+134.76 F(G)

IR = 0.00+1.5 F (G)

MR = 0.27+15.33 F (G)

PSA = 0.022+83.88 F (G)

P = 0.123+6.75 F (G)

ST = -0.016+54.77 F (G)

MV = 0.84+46.17 F (G)

HM Index HM (G):

D = 0.00+1.326 HM (G)

BP = 0.52+287.36 HM (G)

VP = 0.000+2.123 HM (G)

E = 0.057+59.19 HM (G)

FP = 0.313+127.64 HM (G)

IR = 0.00+1.47 HM (G)

MR = 0.176+0.83 HM (G)

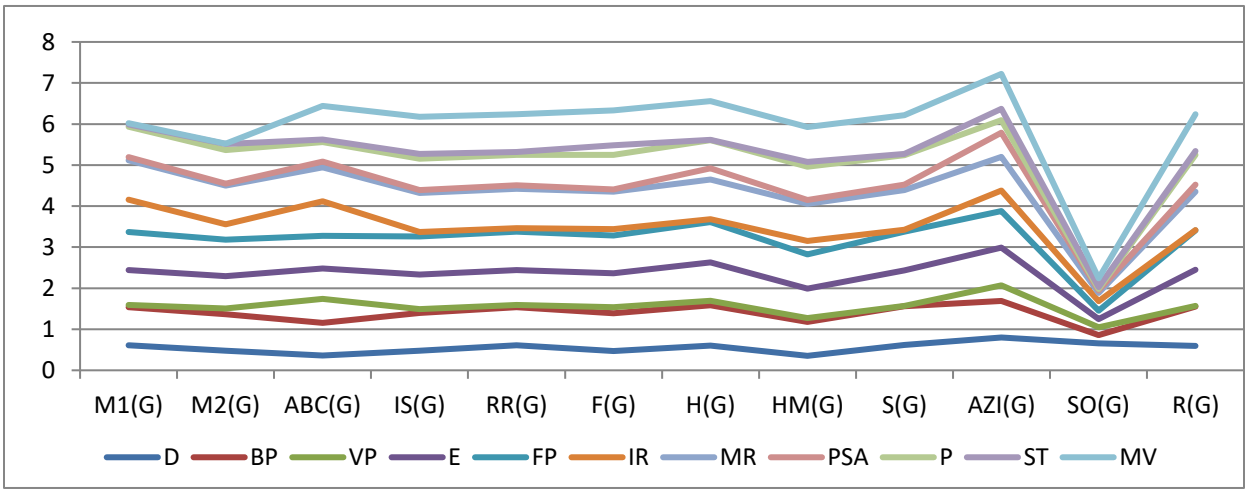
PSA = -0.024+105.66 HM (G)

P = 0.077+2.122 HM (G)

ST = -0.005+52.46 HM (G)

MV = 0.54+0.76 HM (G)

Graph Analysis: Correlation coefficient between physico chemical properties and Topological Indices



Conclusion:

Summarized, the goal of this work is to anticipate significant physical and chemical features of medications used in renal therapy treatment using topological indices. The Table 15 correlation coefficients offer valuable information on the predictive power of these topological indices, which is important for the efficient and cost-effective development of innovative therapeutics with the necessary attributes. Molar Refraction is a useful descriptor in QSPR modelling for understanding and predicting the physical chemical features of medications used to treat hypertension. These strong relationships between Molar Refraction and the topological indices support this. Future research attempts to optimize drug structure to increase desired attributes efficiently might benefit from this understanding, which strongly correlates with M1 (G), 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) with an Excellent squared (r2=0.9) and correlation coefficients (r=0.99).

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