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TWENTY COMPOUNDS INHIBITING EBOLA VIRUS, THEIR PROPERTIES AND DRUG-LIKENESS, AND ANALYSIS OF PROPERTIES FOR IDENTIFICATION OF SIMILAR COMPOUNDS

***Ronald Bartzatt**

University of Nebraska at Omaha, 6001 Dodge Street, Omaha, Nebraska.

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***Corresponding Author**

***Ronald Bartzatt**

University of Nebraska at Omaha, 6001 Dodge Street, Omaha, Nebraska.

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ABSTRACT

Ebola Virus Disease (EVD) is a serious infection with a substantial mortality rate, that is a type of viral hemorrhagic fever that substantially damages blood vessels (causing hemorrhaging), causes neurological disorders, and severe vomiting. Four different Ebola strains have been identified that are able to infect humans. The search and identification of new treatment pharmaceuticals is continuous and ongoing. This study examines 20 compounds that have been shown to inhibit Ebola virus in previous studies. The molecular properties and drug-likeness for each compound is determined and compared among these 20 compounds. This study, utilizing summary statistics and pattern recognition methods, produced a screening-type process by which other similar compounds could be identified for further study. Pattern recognition methods such as neighbor-joining cluster analysis, 95% ellipses, and box plots are utilized to identify underlying relationships among these 20 compounds that are based on their molecular properties. Over all, this study provides a pathway to identify additional new and effective pharmaceuticals for the treatment of EVD. Multiple regression analysis of their molecular properties produced a formula to enable the design of additional effective compounds. The identification and study of new and effective antivirals for the treatment of EVD is a necessary and a vital objective.

KEYWORDS: EBOLA, anti-virus, EVD, hemorrhagic fever.

INTRODUCTION

Ebola virus disease (EVD) is a very dangerous infection of the hemorrhagic inducing Ebola virus, which is designated into the *Filoviridae* family.[1] To date, four types of Ebola virus has been identified, which are: Bundibugyo ebola virus, Sudan ebola virus (significant cause of death), Tai Forest ebola virus (relatively rare), and Zaire ebola virus (the most common cause of morbidity and death).[1,2,3] In addition, investigations have found evidence of the Ebola virus presence in fruit bats located in Bangladesh.[4] The rapid diagnoses of EVD is vital for retaining survival expectations for patients. Clinical diagnosis is accomplished by various methods, to include reverse-transcription polymerase chain reaction (highly reliable), antigen-capture ELISA, ReEBOV antigen rapid test (test for Ebola virus VP antigen), testing for IgM and IgG, and actual isolation of the virus.[5] Clinical intervention of EVD, following rapid diagnosis, also requires knowledge and appropriate treatment of any co-morbidities such as secondary bacterial infections, septic shock, renal failure, internal bleeding, and malaria management if that is associated to the apparent geographical location of infection.[6] It is important for care-providing facilities to provide fluid rehydration, the balancing of electrolytes and metabolism, and management of vomiting, pain, and diarrhea.[6] Also, the isolation and/or removal of all types of infectious vectors is very important.[6]

Clinical treatment of EVD is an ongoing topic of research, drug development, and clinical investigations. The general description of medicament treatment of EBV can incorporate nucleic acid oligomers, antibody defined therapies, and administration of small drug molecules.[7] Intravenous administration of medicaments has been found to appreciably increase survival rates. Interestingly, the patient response to treatment by way of pharmaceuticals, has been observed to be dose dependent of the utilized drug.[7] Clearly, further investigations of this highly lethal viral infection is warranted. The pursuit of effective pharmaceutical agents for clinical application is vital. In addition, the careful evaluation of the mode and manner of pharmaceutical administration cannot be disregarded in pursuit of successful treatment of patients.[7] This study presents 20 compounds that have been previously shown to inhibit Ebola virus. Molecular properties of these 20 compounds are determined utilizing various heuristic platforms available and examined for commonalities and drug-likeness. Summary statistics provide a rapid evaluation frame work for the screening for similar compounds, along with pattern recognition methods that show

underlying relationships and will assist in evaluations thereof.

MATERIALS AND METHODS

Molecular Properties and Modeling

The numerical values for molecular properties (i.e. Log P, polar surface are, molecular weight, number of atoms, molecular volume, number of nitrogen, oxygen, amine groups, and hydroxyl groups), for all compounds can be determined by Molinspiration Chemical Properties Service, Nova ulica 61, SK-900 26 Slovensky Grob, Slovak Republic (www.molinspiration.com/ cgibin/properties) and/or Mcule (mcule.com, Palo Alto California USA). The Mcule support allows the use of SMILES (Simplified Molecular Input Line Entry System) designation of the compounds in pursuit of molecular properties. Depicting molecular structures of compounds was done by ACD ChemSketch Modeling v. 12.01 (Advanced Chemistry Development, 110 Yonge Street, Toronto Ontario, M5C 1T4 Canada).

Statistical Analysis and Prediction

Multiple regression analysis as well as summary statistics (i.e. mean, median, test for normality, standard deviation, minimum and maximum numerical values) was accomplished utilizing Instat Statistical Analysis Package, version 3.06, Sept. 11 2003 (copyright 1992-2003, www. graphpad.com). Pattern recognition analysis by 95% ellipses, that was preceded by non-metric multidimensional scaling, was accomplished utilizing PAST version 2.06 (copyright Oyvind Hammer, D.A.T. Harper, 2011). Nearest neighbor cluster analysis and box plots were accomplished utilizing PAST version 2.06. Determination of path coefficients following Path Analysis, was accomplished utilizing OpenStat version 3 (William G. Miller, copyright September 11, 2008).

RESULTS AND DISCUSSION

Ebola virus is readily passed on to other humans after exposure to infectious body fluids.[1,2,3,8] Ebola virus infection usually shows rapid development and induces high virulence, which can be followed with a high rate of mortality.[1,2,3] For defining an epidemic, it is the acceleration of disease cases that is the definition whether an epidemic is occurring or not, rather than a specific threshold number of cases. By this standard, a rare disease having few cases could be defined as an epidemic, however for a very common disease even a seemingly high number may not be defined as an epidemic.[1,2,3] The study and advancement of small molecule drugs for clinical treatment of EBV is necessary and possesses advantages as a

treatment system due to various merits such as; the possibility of oral administration of the drug, the efficacious discovery of small molecule drugs, effectiveness in targeting the virus entry mechanism, and the potential of small molecule drugs being less susceptible to virus mutations.[8] Generally, small molecule drugs are accepted to be organic compounds having molecular weight less than 900 Daltons.[8] The relatively smaller molecular weight has several advantages, including: ease of oral administration, ease of passage through cell membranes, being substantially stable at room temperature, the manufacture of which is generally considered cost effective, and do not require a temperature controlled supply chain. Considerable amount of work has been completed identifying small molecule drugs for the clinical treatment of EVB.[8] In addition, further studies have been accomplished to examine the molecular properties, molecular structure, drug-likeness, and commonalities within this class of compounds.[9,10,11] Previous studies have compiled a library of organic compounds that have been shown to inhibit the Ebola virus to varying extent and showing quite diverse molecular structures.[8] Further investigation of these compounds is certainly warranted, and this includes the analysis of the molecular structures, properties, drug-likeness, and feasibility of clinical use. Fortunately, a substantial amount of progress has been made in understanding the drug action and the relation of the molecular framework for an effective clinical pharmaceutical.[12] Various aspects of the molecular skeleton of drugs can be understood to play a substantial role in the drug-likeness (evaluation of absorption, distribution, metabolism, excretion, and toxicity). A compound will have favorable oral bioavailability if it violates no more than one of the following criteria, known as the Rule of 5 (RO5): 1) Has no more than 5 hydrogen bond donors (total of -OH and -NHn); 2) Has no more than 10 hydrogen bond acceptors (total of nitrogen and oxygen atoms); 3) Has molecular mass less than 500 Daltons; 4) A calculated Log P not greater than 5.0.[12] It follows, that each atom within the molecular structure of the drug that are vital for the pharmaceutical action of the compound, are also part of various properties such as polar surface area, rotatable bonds, molecular volume, molecular weight, etc.

The molecular framework of 20 compounds that inhibit Ebola virus are shown in Figures 1, 2, 3, and 4. With each compound structure is presented the SMILES notation (Simplified Molecular Input Line Entry System). This group of compounds are diverse in molecular structure, however all have molecular weight less than 900 Daltons, and therefore are considered small molecules for drug considerations (thereby, having the benefits for clinical

use as described previously). Among the molecular framework of these 20 compounds are found carbonyl groups, amine groups, hydroyl groups, aromatic rings, methoxy groups, carboxylic acid, and various chains of carbon (see Figures 1,2,3,and 4). Although the molecular framework of these 20 compounds are quite diverse, the numerical values of the molecular properties can be determined by use of the heuristic methodologies and platforms that been shown to be remarkably useful and accurate (see MATERIALS AND METHODS).[13]

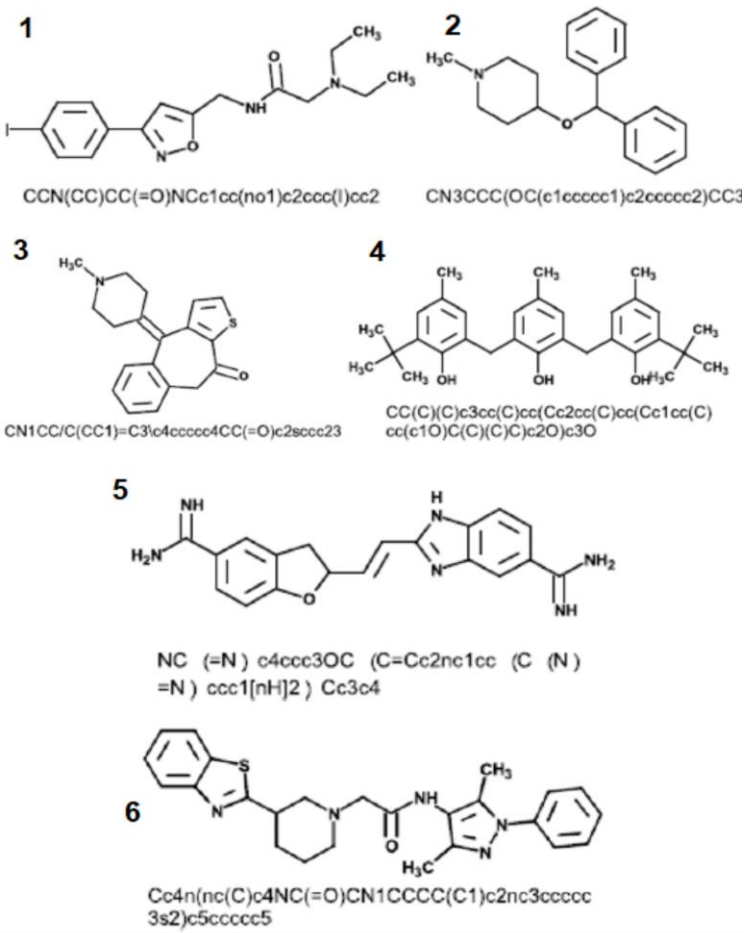

Figure 1: Anti-Ebola compounds having molecular weight ranging from 281.4 Daltons (#2) to 460.66 Daltons (#4). A variety of structures are evident, having aromatic rings, methyl groups, amide groups, hydroxyl groups, and carbonyl groups.[8] SMILES notation for each compound is displayed.

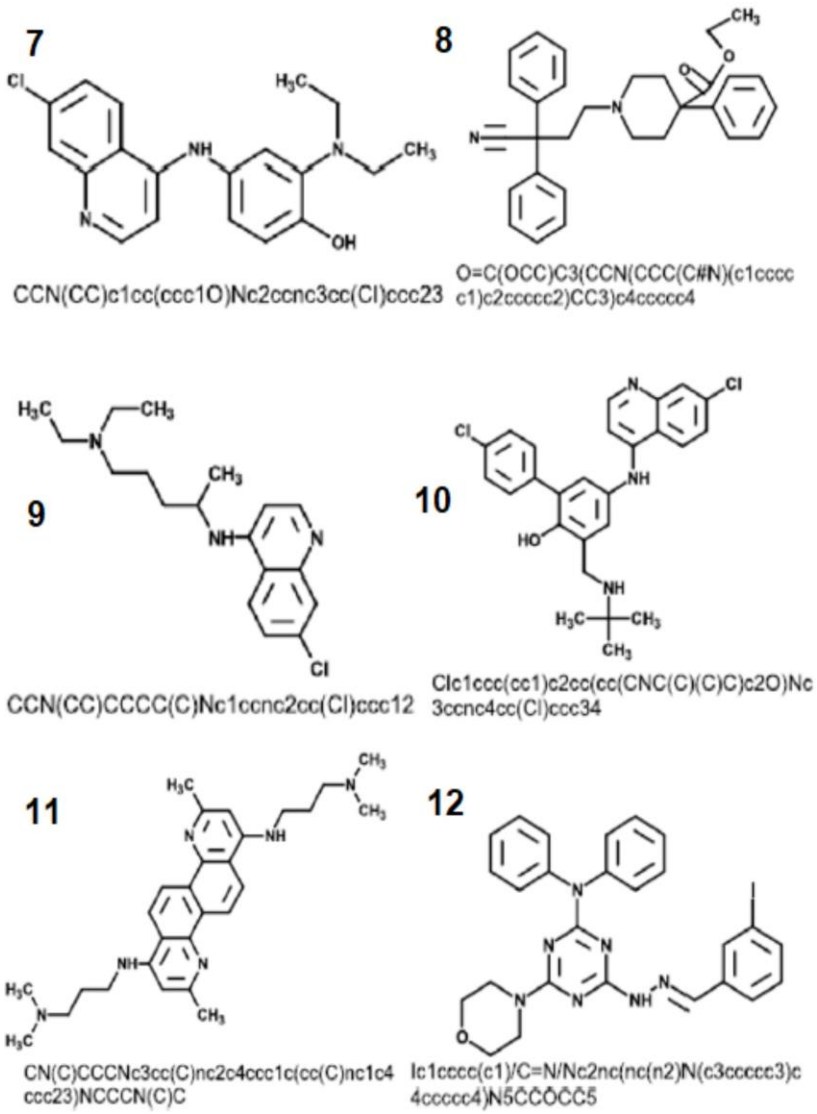

Figure 2: Anti-Ebola compounds having molecular weight ranging from 319.88 Daltons (#9) to 577.43 Daltons (#12). A variety of structures are evident, with components such as aromatic rings, methyl groups, amine groups, hydroxyl groups, and ester group.[8] SMILES notation for each compound is presented.

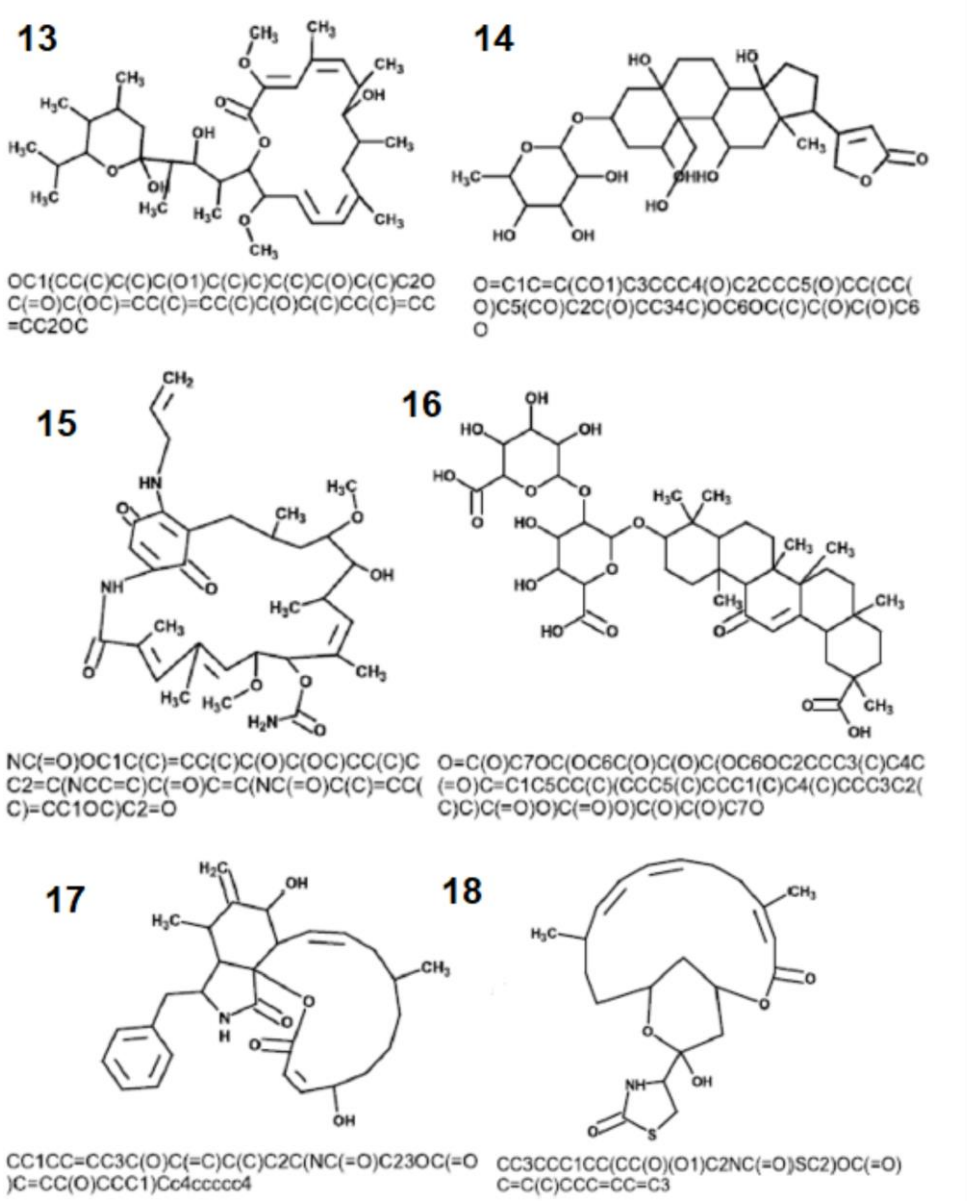

Figure 3: Anti-Ebola compounds having molecular weight ranging from 421.56 Daltons (#18) to 822.94 Daltons (#16). A variety of structures are evident, having components such as aromatic rings, methyl groups, carboxylic acid groups, hydroxyl groups, and carbonyl groups.[8] SMILES notation for each compound is shown.

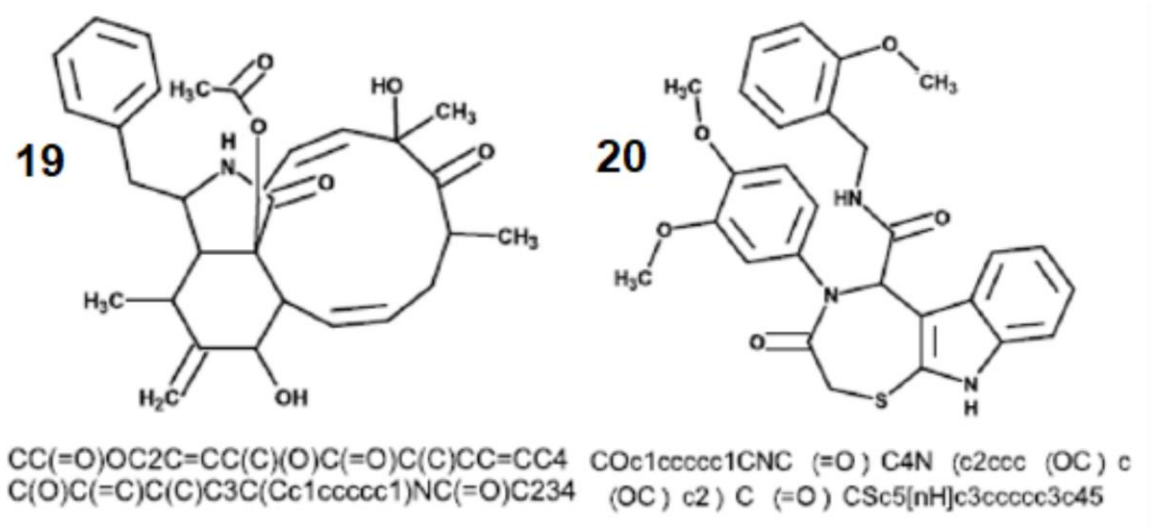

Figure 4: Anti-Ebola compounds having molecular weight ranging from 507.63 Daltons (#19) to 517.61 Daltons (#20). A variety of structures are evident such as aromatic rings, methyl groups, hydroxyl groups, methoxy groups, and carbonyl groups.[8] SMILES notation for each compound is displayed.

Even with the diverse molecular framework of these 20 compounds, it is still possible to understand and identify commonalities based on the numerical values of the molecular properties. Consequently, the screening methodologies, such as the Rule of 5, may be applied in order to identify compounds likely to be successful as a clinical pharmaceutical tool. To this end, nine molecular properties, useful in establishing drug-likeness and making comparison among these 20 compounds, are shown in Table

1. Numerical values of molecular properties can be efficiently acquired by use of the various heuristic platforms currently available (see MATERIALS AND METHODS). The properties for these 20 anti-Ebola compounds are listed in Table 1, these properties are utilized often to understand drug-likeness as well.[12,13] Altogether, these properties indicate that most of these 20 compounds have favorable drug-likeness based on the Rule of 5 (RO5).[12] Wherein, most of the compounds have merely one violation of RO5 or zero violations (see Table 1). The exceptions to the RO5 criteria are only compounds 12, 14, 15, and 16, in which there are two or more violations of RO5 (see Table 1).

The summary statistics for properties listed in Table 1 are compiled and shown in Table 2. Summary statistics communicates the condensed version of data and a large amount of information as succinctly as possible.[14,15] Summary statistics presents the central tendency,

statistical dispersion, the shape of the distribution, and measure of statistical dependence on individual variables.[14,15] Essentially, summary statistics provides an effective early step to analyze data and enables informed decision making and enable further analysis for purposes of data comparison, recognition of trends, the identification of anomalies and outliers.[14]

Table 1: Molecular Properties of 20 Compounds Inhibiting Ebola Virus.

Compound	Log P	Polar Surface Area (A^2)	Number of Atoms	Molecular Weight	Oxygen Nitrogen Atoms	Number of -OH & -NH_n	Rotatable Bonds	Volume (A^3)	Rule of 5
1	3.58	58.37	22	413.26	5	1	7	301.35	0
2	3.16	12.47	21	281.4	2	0	4	286.8	0
3	3.48	20.31	22	309.43	2	0	0	284.23	0
4	8.93	60.68	34	460.66	3	3	6	466.57	1
5	0.47	137.67	26	346.39	7	7	4	306.84	1
6	3.77	63.05	32	445.59	6	1	5	405.90	0
7	5.38	48.38	24	341.84	4	2	5	308.75	1
8	5.96	53.34	34	452.60	4	0	9	440.81	1
9	5.00	28.16	22	319.88	3	1	8	313.12	1
10	7.67	57.17	32	466.41	4	3	8	409.58	1
11	4.72	56.31	34	458.65	6	2	10	458.26	0
12	6.6	78.78	35	577.43	8	1	7	436.37	2
13	4.8	114.69	44	620.87	8	3	7	630.37	1
14	-2.18	206.6	41	584.66	12	8	4	520.54	3
15	2.11	166.29	43	599.73	11	5	7	570.06	2
16	1.97	267.04	58	822.94	16	8	7	741.93	3
17	4.11	98.86	35	479.62	6	3	2	480.90	0
18	3.52	84.86	29	421.56	6	2	1	391.39	0
19	2.89	112.93	37	507.63	7	3	4	479.11	1
20	3.84	92.9	37	517.61	8	2	7	453.35	1

Table 2: Summary Statistics of Molecular Properties For 20 Compounds Inhibiting Ebola Virus.

Statistic	Molecular Weight	Log P	Polar Surface Area (A^2)	Number of Atoms	Oxygen & Nitrogen	Number of -OH & -NHn	Rotatable Bonds	Volume (A^3)	Rule of 5
Mean	471.41	3.99	90.943	33	6	3	6	434.31	1
Standard Deviation	128.73	2.44	63.64	9	4	3	3	120.76	1
Minimum	281.40	-2.18	12.47	21	2	0	0	284.23	0
Maximum	822.94	8.93	267.04	58	16	8	10	741.93	3
95% Confidence Interval	411.16 to 531.66	2.85 to 5.13	61.16 to 120.73	29 to 37	5 to 8	2 to 4	4 to 7	377.80 to 490.83	0 to 1

Multiple Regression Analysis of Molecular Properties

Multiple regression analysis will model the relationships between one dependent variable (molecular weight descriptor in this study) to multiple independent variables (remaining descriptors, see Table 1). The model can be used to predict new observations, formulate understanding of the factors that influence a target variable, and to evaluate the strength (i.e. influence) of independent variables.[14,15] Molecular properties of Table 1 are analyzed, with the model outcome presented below for the dependent variable MW (molecular weight). The independent variables are Log P, PSA (polar surface area, units are Angstroms^2), Natoms (number of atoms), nON (number of oxygen & nitrogen atoms), nOHNHn (number of hydroxyl and amine groups), Rotatable Bonds, Volume (molecular volume of molecule, units are Angstroms^3), and RO5 (violations Rule of 5).

MW= 68.767 + 13.226(Log P) + 0.5418(PSA) + 1.202(Natoms) + 20.787(nON) - 12.244(nOHNHn) - 0.5362(Rotatable Bonds) + 0.3635(Volume) + 6.939(RO5)

The regression model accounts for 98.02% of the variance in the molecular weight (R^2= 0.9802). Within the model, the most significant contributions come from values of the constant (*P=.041*), Log P (*P=.014*), and nON (*P=.032*). The model can be utilized to predict potential effective molecules following calculation of molecular properties, inserted into position of these variables, and having coherent and consistent outcome to this overall group of 20 compounds.

Utilization of Pattern Recognition Methods

Application of pattern recognition methods is widely used for data mining in areas of science.[14,15] Here a large amount of data can be analyzed to extract trends and reduce numerical dimensionalities into more manageable, but very informative representations.[14,15] Figure 5 presents outcome of neighbor-joining cluster analysis of properties in Table 1. This cluster analysis using single linkage (minimum distance between any individual pair of members, one from each cluster, joining the clusters having closest observations) and Euclidean distance (the straight line distance between two points).[15] In Figure 5, the 20 compounds are organized such that, based on molecular properties, the compounds most similar to each other will be grouped in the same cluster of compounds, yet have their distance from each other indicated by the length of the segment connecting them within the cluster (see Figure 5). Here in Figure 5, there exists three super clusters having: 1)

Compounds 4 and 11; 2) Compounds 2, 3, 9, 7, 5, 1, 18, 6, 10, and 8; and 3) Compounds 17, 20, 19, 12, 14, 15, 13, and with 16 an extreme and distinct compound, that will also be an outlier in 95% ellipses. Substantial resolution and differentiation of these compounds can be accomplished by use of neighbor-joining cluster analysis, that is based on the molecular properties listed in Table 1. This allows further comparison, the recognition of underlying relationships (including similarities), and enable identification of the optimal molecular properties.

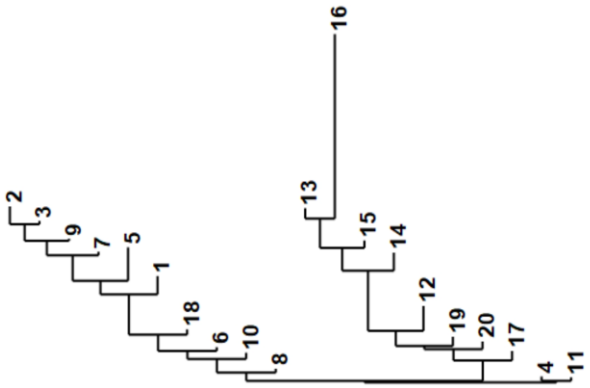

Figure 5: Neighbor-joining cluster analysis (Single Linkage, Euclidean distance) for all 20 compounds that inhibit Ebola virus (see Table 1). Distance between objects (compounds) is indicated by length of leaf segment. Compound 16 is an extreme observation.

Further elucidation of the underlying relationships of this group of 20 compounds can be recognized by use of 95% ellipses, an analysis which will enclose 95% of data points, show dispersion of the data points, identifies trends, reveals outliers, and identifies central tendencies.[14,15] In Figure 6, the compound 16, lies outside the ellipses and therefore can be identified as an outlier (or extreme observation). Also, identifiable are the bulk of the compounds around the origin (see intersection of zero point for x-axis and y-axis), including compounds 4, 6, 8, 10, 11, 12, 17, 18, and 19. Within the boundaries of the ellipses, new and predicted compounds of similar activity are expected to fall, a useful tool for identifying similar potential anti-viral agents. The increased size of this ellipses suggests higher variability within the molecular properties, this assertion supported by the summary statistics of the molecular properties (see Table 1 and Table 2). The elongation of the ellipses suggests linear relationships exists within the properties of these 20 compounds (see Table 1 and Table2).

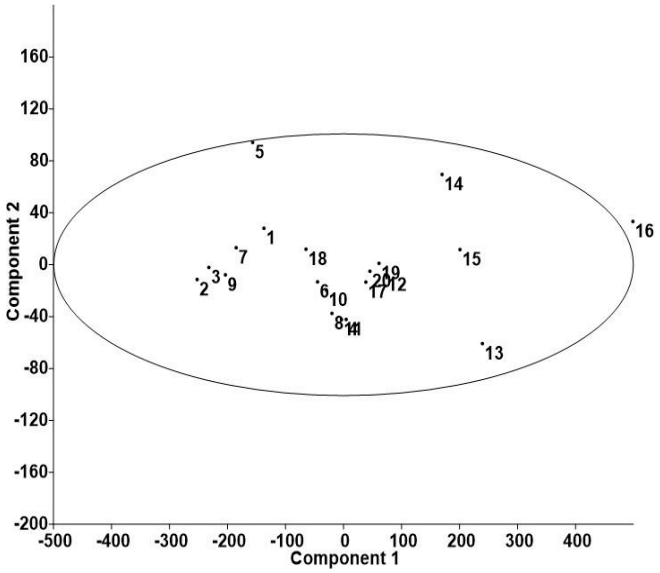

Figure 6: Shown is 95% ellipses enclosing 95% of data points, following non-metric multidimensional scaling of properties compiled in Table 1. This visualizing shows where 95% of the data points are enclosed and prediction where new objects (compounds) similar to this group is likely to fall. The elongated spread indicates strong linear relationships within the data, with compound #16 shown as an outlier from all other compounds.

Box plots are a useful tool for pattern recognition within multiple datasets having multivariate cases/objects. The visual presentation in the form of box plots allows the comparison among different groups as well as summarizes such statistics such as minimum, maximum, media, variability, skewness, and outliers.[14,15] Shown in Figure 7, are the box plots for molecular properties presented in Table 1. Summary statistics for all properties are shown in Table 2. Looking at Figure 7, the numerical values for Log P, number of atoms (Natoms), number of oxygen & nitrogen atoms (nON), number of - OH and -NHn (-OH & -NHn**),** rotatable bonds (Rot Bonds), molecular volume (Volume) and violations of Rule of 5 (RO5) are narrow in range and restricted in numerical spans, despite the considerably broader variation in values for polar surface area (PSA), molecular weight (MW) in particular, and molecular volume (Volume). Numerical range for MW is quite broad (281.40 Daltons to 822.94 Daltons) considering the limitations in range for properties listed above, suggesting the carbon skeleton for this group of compounds are varied and expansive in framework. Consequently, the molecular volume (Volume) with range 284.23 Angstroms^3 to 741.93 Angstroms^3 will follow in variation and is visible in the Figure 7. Interestingly, although the polar surface area (PSA) of compounds is summation of oxygen and nitrogen atoms, the

range in PSA is 12.47 Angstroms^2 to 267.04 Angstroms^2, giving a broad range of PSA even though nON and (-OH & -NHn) are small, narrow, and constrained (see Figure 7).

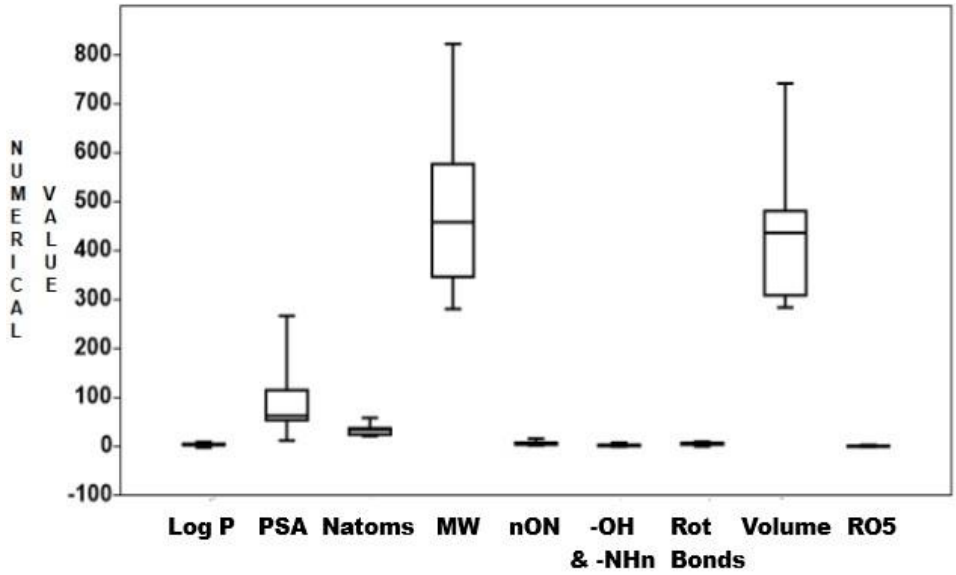

Figure 7: Box plot of properties (see Table 1) labeled Log P, PSA (polar surface area), Natoms (number of atoms), MW (molecular weight), nON (number of oxygen and nitrogen atoms), number of hydroxyl and amine groups (-OH & -NHn), Rot Bonds (rotatable bonds), molecular volume (Volume), and Rule of 5 (RO5).

Path analysis (or causal modeling), is a special case of structural equation modeling that is focused on causality, it is considered a confirmatory technique, and describes directed dependencies among a set of variables (molecular properties in this study).[16,17] Numerical values of path coefficients, along with positive (+) or negative sign (-), can be interpreted as to the strength and direction of dependency of the molecular properties to molecular weight.[16,17] Table 3 presents path coefficients for the caused variable (molecular weight for this study) and causing variables (all remaining molecular properties), where size of numerical value and sign (+ or -) relates the causal relationship. A positive value (+) indicates an increase in the dependent variable (molecular weight in this study) with an increase of the designated independent variable (any of the remaining properties). A negative value (-) indicates an inverse relationship of the dependent variable to the independent variables. The results of causal modeling indicates that number of oxygen & nitrogen atoms (coefficient = 0.568) and molecular volume (coefficient = 0.341) have the strongest causality, followed by polar surface area (coefficient = 0.268) and Log P (coefficient = 0.251). Wherein the strong positive value shows a direct relationship to molecular weight (increase in either property

results in increase in molecular weight). Interestingly, the number of rotatable bonds (coefficient = -0.011) and number of -OH and -NHn (coefficient = - 0.235) have an inverse causal effect on molecular weight.

Table 3: Causal Model Path Coefficients To Molecular Weight.

Summary of Causal Models		
Causing Variable	**Variable Caused**	**Path Coefficients**
Log P	Molecular Weight	0.251
Polar Surface Area	Molecular Weight	0.268
Number of Atoms	Molecular Weight	0.086
Oxygen & Nitrogen Atoms	Molecular Weight	0.568
Number of -OH & -NHn	Molecular Weight	-0.235
Rotatable Bonds	Molecular Weight	-0.011
Volume	Molecular Weight	0.341
Rule of 5	Molecular Weight	0.051

Modification of molecular structure is a vital aspect of drug development, in that beneficial activity is accentuated and undesirable side-effects are reduced.[18] This study presents the clear and object diversity of molecular structure and attending molecular properties for a group of compounds known to inhibit Ebola virus. Clearly the varied framework of their molecular structure warrants study and analysis. From molecular properties, some interesting activity of compounds can be presumed, for some of these 20 compounds the polar surface area is less than 90 Angstroms^2 and thus favorable for crossing the blood-brain barrier (these are 1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, and 18).[19,20] In addition, further studies have shown that compounds having polar surface area less than 140 Angstroms^2 have favorable cell membrane permeation.[21] Of these 20 compounds, the following have polar surface area less than 140 Angstroms^2: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 17, 18, 19, 20. Molecular properties will continue to influence the identification and success of perspective clinical pharmaceuticals. All the compounds presented in this study are considered to be small molecules. Small molecule drugs have many advantages for treatment of EVD, which includes the targeting of multiple stages of the virus life cycle, inclusive of the transcription, replication, egress, and entry of the virus.[22] The continued study of small molecules to discover drugs for the successful clinical treatment of EVD is ongoing and necessary.

CONCLUSION

This study has shown that 20 compounds previously demonstrated to inhibit Ebola virus, have quite diverse molecular frameworks, however, various drug-likeness molecular properties are firmly restricted in numerical values. Summary statistics showed that the molecular properties broadest in range were molecular weight, polar surface area, and molecular volume. The molecular framework of these 20 compounds are considerably diverse, having carbon chains, aromatic rings, hydroxyl groups, carbonyl groups, methoxy groups, ester groups, amine groups, and methyl groups. All compounds showed favorable oral bioavailability according to the Rule of 5, except for compounds 12, 14, 15, and 16. Many of these 20 compounds have polar surface area less than 90 Angstroms^2, favorable values for crossing the blood-brain barrier (these are 1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, and 18). Furthermore, many of these compounds have polar surface area less than 140 Angstroms^2, which is a favorable value for cell membrane permeation. The following have polar surface area less than 140 Angstroms^2: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 17, 18, 19, 20. Pattern recognition analysis identified underlying relationships according to their molecular properties, revealing compound 16 is an extreme outlier. Neighbor-joining cluster analysis indicated that compounds 4 and 11 are most similar to each other, whereas compounds 2, 3, 9, 7, 5, 1, 18, 6, 10, and 8 together most similar to each other. The remaining compounds 13, 15, 14, 12, 19, 20, and 17 are separate from all the rest. Molecular properties strongly influence the identification and success of potential clinical medicaments.

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