Math Notes: Functional Relationships in the Correlation Structure for Polar Area, Complexity and H Bond acceptor Count from Tanimoto Similarity of Antibiotic Protein Synthesis Inhibitors

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The Mathematical Learning Space Research Portfolio: Math Note 3

Abstract: More than 2.8 million people become infected with antibiotic resistant bacteria each year. For example, a collection of Gram-positive bacteria difficult-to-treat infections use ribosomal protection such that antibiotics that cannot bind to the ribosome. Several chemical extracts from the genus Liquidambar was examined with a selection of 3-phenylpropyl cinnamate Density and Correlation Structure for Polar Area, Complexity and H Bond acceptor count for a Tanimoto Similarity of 3-phenylpropyl cinnamate. In the three molecular properties, a nonlinear relationship was established based on an N=1000 for each of the bivariate relationships. Puromycin is an antibiotic protein synthesis inhibitor for premature chain termination during translation was examined with the NCI-60 cell lines for 40S ribosomal proteins RPS2 RPS7 and RPSA none of the correlations are significant with the compound. However, differences were found in the bivariate relationships of the molecular properties between the two compounds was observed.

Keywords: Environmental Science Antimicrobial resistance Ecological genetics 3-phenylpropyl cinnamate Gram-positive bacteria

1 Introduction

Ecological genetics in environmental science involves the study of the increases of antimicrobial resistance caused by increased prescription and the dispensing of antibiotic drugs in developing countries with more than 700,000 to several million deaths result per year. For example, each year in the United States, at least 2.8 million people become infected with bacteria that are resistant to antibiotics and at least 35,000 people die as a result. [2] There are five main mechanisms by which bacteria exhibit resistance to antibiotics are: (1) Drug inactivation or modification (2) Alteration of target- or binding site, (3) Alteration of metabolic pathway. (4) Reduced drug accumulation and (5) Ribosome splitting and recycling. [2]

In (2) bacterial species have ribosomal protection proteins that protect the bacterial cell from antibiotics that target the cell's ribosomes to inhibit protein synthesis. The algorithm involves the binding of the ribosomal protection proteins to the ribosomes of the bacterial cell with a changes in its conformational shape and permits the ribosomes to continue synthesizing proteins essential to the cell and antibiotics cannot bind to the ribosome to inhibit protein synthesis. [2]

For example, Methicillin-resistant Staphylococcus aureus (MRSA) is a collection of Gram-positive bacteria difficult-to-treat infections in humans. Antibacterial chemical extracts from various species of the sweetgum tree (genus Liquidambar) can inhibit MRSA such as (a) cinnamic acid, (b) cinnamyl cinnamate, (c) ethyl cinnamate, (d) benzyl cinnamate, (e) styrene, (f) vanillin, (g) cinnamyl alcohol, (h) 2-phenylpropyl alcohol, and (i) 3-phenylpropyl cinnamate. [3]

Figure 1 provides the molecular arrangement for 3-phenylpropyl cinnamate.

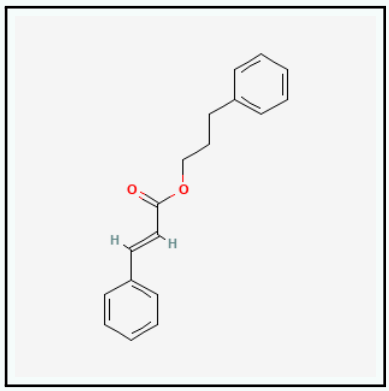

Figure 1: 3-phenylpropyl cinnamate for CID5320530 [470]

2 Results

Consider the N=1000 similarities for 3-phenylpropyl cinnamate with features based in intervals [] , the molecular weight is [100,800], rotatable bond count [1,35], the heavy atom count [13,53], the H Bond donor count [0,1], the H Bond acceptor count [2,23], Polar area is [20,130], the Complexity [100,1300], the XLogp [1,18] and the creation date is from [2005,2021]. [470] Figure 2 presents the Density and Correlation Structuere for Polar Area and Complexity for Tanimoto Similarity of 3-phenylpropyl cinnamate.

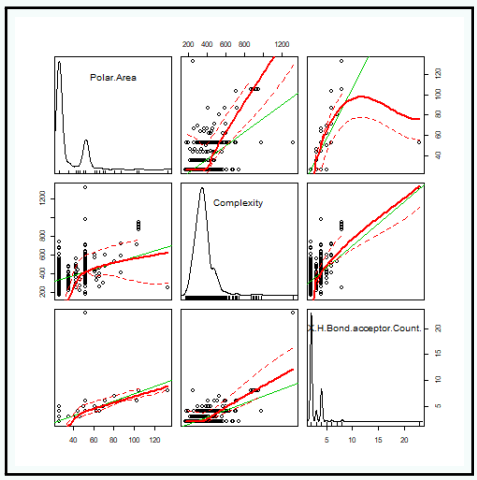

Figure 2: Density and Correlation Structure for Polar Area, Complexity and H Bond acceptor count for Tanimoto Similarity of 3-phenylpropyl cinnamate. [1000]

Consider Puromycin is an antibiotic protein synthesis inhibitor and causes premature chain termination during translation presented in Figure 3. [5].

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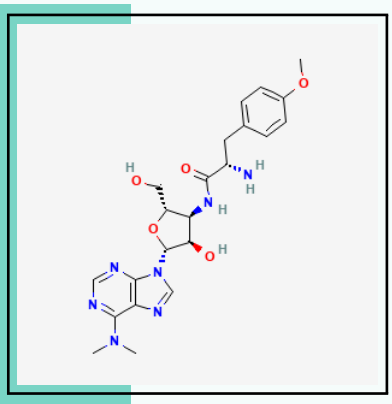

Figure 3: Puromycin is an antibiotic protein synthesis inhibitor [470]

Figure 4 has the Density and Correlation Structure for Polar Area, Complexity and H Bond acceptor count for Tanimoto Similarity of Puromycin.

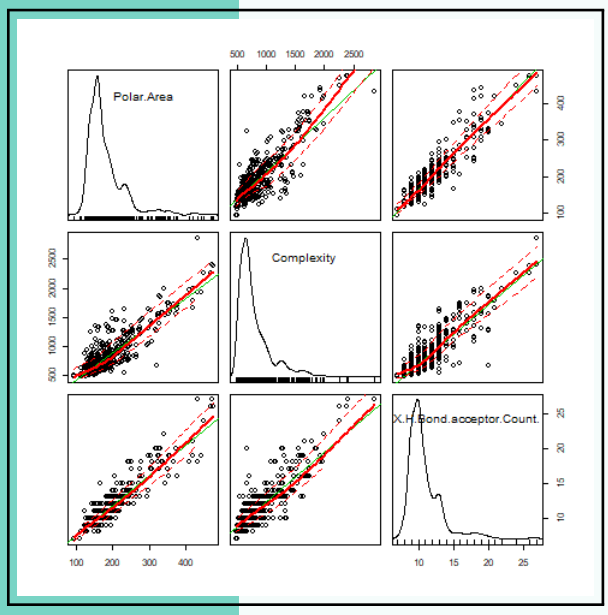

Figure 4: Density and Correlation Structure for Polar Area, Complexity and H Bond acceptor count for Tanimoto Similarity of Puromycin. [1000]

Here a linear relationship is the result of the pairings. For the NCI-60 cell lines, Table 1 has the expression result correlations with p and q values for puromycin with 40S ribosomal proteins RPS2 RPS7 an RPSA [6]. Here none of the correlations are significant with the compound for all cell lines. [1006]

	COR	PVAL	QVAL
RPS2	0.10	0.51	0.77
RPS7	-0.12	0.44	0.77
RPSA	0.03	0.86	0.86

Here Table 1 has the cell lines from NCI-60.

1	BR:MCF7	BR:MDA_MB_231	BR:HS578T	BR:BT_549
2	BR:T47D	CNS:SF_268	CNS:SF_295	CNS:SF_539
3	CNS:SNB_19	CNS:SNB_75	CNS:U251	CO:COLO205
4	CO:HCC_2998	CO:HCT_116	CO:HCT_15	CO:HT29
5	CO:KM12	CO:SW_620	LE:CCRF_CEM	LE:HL_60
6	LE:K_562	LE:MOLT_4	LE:RPMI_8226	LE:SR
7	ME:LOXIMVI	ME:MALME_3M	ME:M14	ME:SK_MEL_2
8	ME:SK_MEL_28	ME:SK_MEL_5	ME:UACC_257	ME:UACC_62
9	ME:MDA_MB_435	ME:MDA_N	LC:A549	LC:EKVX
10	LC:HOP_62	LC:HOP_92	LC:NCI_H226	LC:NCI_H23
11	LC:NCI_H322M	LC:NCI_H460	LC:NCI_H522	OV:IGROV1
12	OV:OVCAR_3	OV:OVCAR_4	OV:OVCAR_5	OV:OVCAR_8
13	OV:SK_OV_3	OV:NCI_ADR_RES	PR:PC_3	PR:DU_145
14	RE:786_0	RE:A498	RE:ACHN	RE:CAKI_1
15	RE:RXF_393	RE:SN12C	RE:TK_10	RE:UO_31

Figure 5 has the histogram of expressions for both (a) drugs (b) genes based on all cell lines.

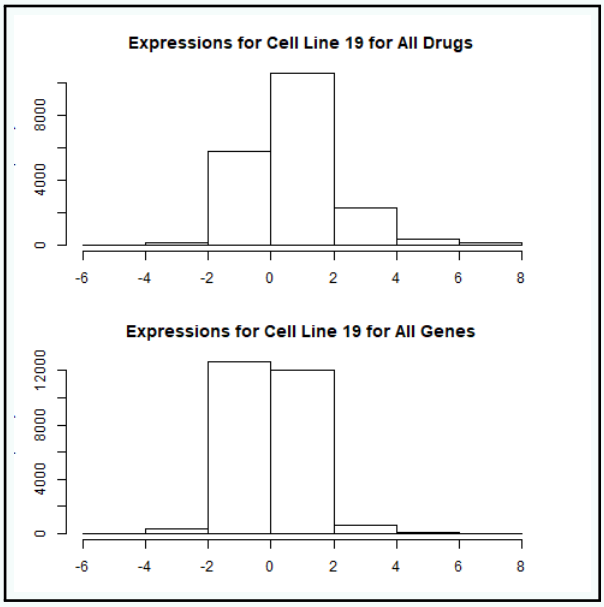

Figure 5: Histogram for (a) drugs and (b) genes [1000]

For an n * p data matrix (or data frame) x, compute the "outlyingness" of all n observations. Outlyingness here is a generalization of the Donoho-Stahel outlyingness measure, where skewness is taken into account via the medcouple, Figure 6 has the histograms for both (a) 595 and (b) 214 outliers.[1010]

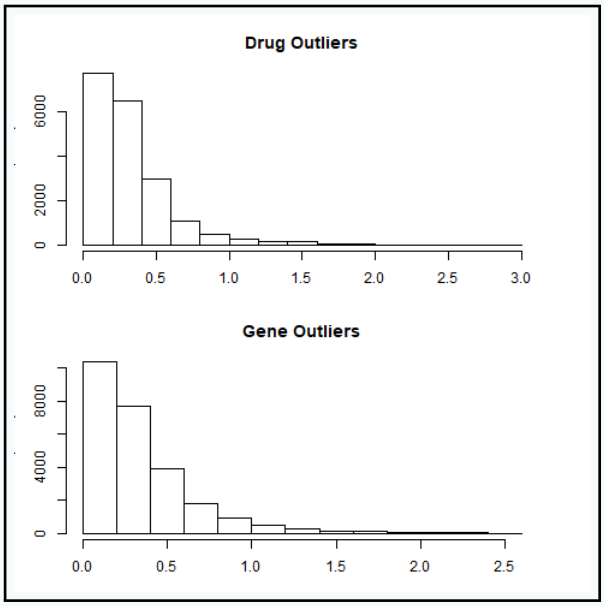

Figure 6: Histogram for (a) and (b) [1000]

3 Conclusion

Several chemical extracts from the genus Liquidambar was examined with a selection of 3-phenylpropyl cinnamate Density and Correlation Structure for Polar Area, Complexity and H Bond acceptor count for Tanimoto Similarity of 3-phenylpropyl cinnamate. Based on a sample of N=1000, nonlinear relationship in the correlation for each of the bivariate relationships. Puromycin is an antibiotic protein synthesis inhibitor for premature chain termination during translation. [5]. For the NCI-60 cell lines, puromycin with 40S ribosomal proteins RPS2 RPS7 and RPSA none of the correlations are significant with the compound for all cell lines. Differences were found in the bivariate relationships between the two compounds. This information can be useful in the construction of chemical scales for machine learning.

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