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Modelling and Characterization of Amino Acids Using MOS Technology

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***Abstract*—Electrical Circuit Modeling of Amino acid based on their structural and chemical properties using electrical R, C components has been reported in this paper. The components are designed by Metal-Oxide-Semiconductor (MOS) technology. Hydrophilic and hydrophobic property of amino acid is only considered here for their characterization. The electrical circuit is realized both by passive and active mode and analyzed the simulated results . A Comparison has been drawn based on response of active and passive model .**

***Keywords*—Amino Acid; Genomics; Modelling; MOS; Protein;**

I. INTRODUCTION

Amino acids are the main building blocks or chemical units for proteins. The genes of DNA are responsible for the creation of amino acids [1]. There are twenty amino acids joined together by peptide bonds to form the basic structure of proteins present in every living cells, lack of which can cause indigestion, depression, physical disorders, etc. Amino acids consist of carbon compounds, contain two functional groups: an amino group (NH_2) and a carboxylic acid group (COOH). A side chain (r) attached to this compound gives each amino acid a unique set of characteristics due to its different component in the side chain. Only Proline has a slightly different structure as the "r" group is bent into a circle to attach itself with nitrogen in place of one of the hydrogen atoms. Fig. 1 illustrates the basic structure of amino acid.

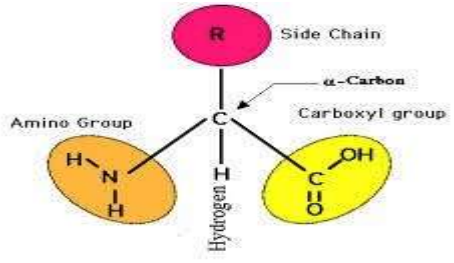

Fig1. Basic structure of amino acid

In genomics, modelling of DNA and protein is a very recent trend to learn their structure and functionality. Different complex network approaches have been proposed by several authors to model DNA/RNA, amino acid and protein structure [2-7]. Marshall [2], [3] has developed resistor capacitor ladder network for DNA/RNA strings and amino acid strings. The passive analog electrical circuits for protein structure have been modelled by Sampath [4].

The secondary structure and the secondary structure linkages have been modelled using resistor, capacitor and inductor by Marshall [5].

In [6], Hodzic et al. have developed a PSpice model to study the electrical behaviour of DNA molecules. It has been understood from various literature survey that the property and structure of amino acid is very important as twenty amino acids are coded by DNA to form proteins. The structure of protein and its property is also important for designing structure based drugs and prediction of genetic disease [7].

All of the amino acids already designed using passive R, L, and C component which is presented in [8]. Here the authors presented the amino acid modelling based on MOS technology, considering power consumption and chip area. Realizing the importance of amino acids in the medical society, we modelled each acid using electrical component R, C which are designed by MOS technology and study their electrical response to characterize them based on their amplitude values at different frequencies.

Gene is a segment of DNA that contains genetic code, translated into twenty amino acids. These amino acids are essential to form antibodies, to protect from bacteria and viruses; they are part of the enzyme and hormonal system; carry oxygen throughout the body and are part of all muscular activity [9]. Researchers have classified the amino acids in different ways. Amino acids are generally categorized based on the structure and property i.e. physicochemical property of their side groups. Proteins are combination of various amino acids and the properties of the side chains determine the properties of the protein. The side chain (r), functional group of amino acids is distinctive which defines a particular amino acid. As the characterization of amino acids is depends on side chain (r) property, the authors have given more importance on side chain while designing amino acids using MOS technology. Generally the amino acids are categorized according to their hydropathy index [10], volume, water affinity property. Here we concentrate only on the hydropathy index value for categorizing the amino acids. The list of twenty amino acids and their chemical structure are depicted in Table.1.

The paper is organized into following sections: Section 1 illustrates brief introduction of amino acids; section 2 describes the method for the electrical circuit modelling of amino acids. In section 3, discussions have been made based on the results obtained and finally, conclusion is drawn in section 4.

II. ELECTRICAL CIRCUIT MODELING OF AMINO ACIDS USING MOS

In this section, we described the method of electrical circuit modelling and characterization of amino acids. All of the amino acids modelled by R, C component which are designed by active MOS for considering low power consumption and getting compact layout area. MOS are restricted to operate in linear region for designing the active resistor (R). Drain and source terminal tied together for realization of a active capacitor. Cgd, capacitance measured by gate to drain and Cgs, the capacitance measured by gate to source.

As in the basic structure of amino acids contain a central alpha-carbon to which the carboxyl group (COOH), amino group (NH_2) and the variable side chain (r) are attached, an attempt has been made to realize the electrical circuit model of amino acid based on its structure using electrical component R and C. The generalized model of an amino acid is consist of three distinct circuits, two parallel circuits one of which represent the carboxyl and other represent the amino group called backbone structure, common for all amino acids except Proline and the third which is connected in series with the backbone structure represents the side chain.

We have modelled the carboxyl (COOH) by two series resistor (R) and the amino group is represented by two parallel capacitor (C). The alpha-carbon and hydrogen atom is taken as a node. The non reactive group element is designed by resistor and reactive group elements are designed by different combination of resistor and capacitor.
The side chain components of the amino acids are modelled as follows:
Carbon ≡ R, Hydrogen ≡ C, Oxygen ≡ R || C, Nitrogen ≡ (C||C) + R and Sulphur ≡ (R||R)+C .
And for calculation of R & C: We calculated resistance in linear region R_{ds} (drain to source resistance) using the following Equation 1.

$$R_{ds} = 1/\mu CoxW/L\ (V_{gs}- V_{th}) \quad \text{---------- (1)}$$

Where, t_{ox} (Oxide thickness) = $9.6*10^{-9}$, μ_n (Mobility) = 546.2, €o= $8.854*10^{-14}$, V_{th} (threshold voltage) = 0.6 and V_{gs} (gate-source voltage) kept at 2V.

The calculated value of R_{ds} using Equation (1) is 0.13 Ω; and as gate-drain tied together
$$Cgs = Cgd = CGSO.W=CGDO.W \quad \text{---------- (2)}$$

Where CGSO = Overlap gate to source capacitance and CGDO = Overlap gate to source/drain capacitance. For tanner version 16, CGSO = CGDO = $3.0515*10^{-10}$, length of MOS (L) = 500 nm and width of MOS (W) = 2.5µ. The calculated value of oxide capacitance obtained from Equation (2) is Cgs = Cgd = 0.75 fF.

All amino acids are designed using the calculated value of R and C. Amplitude response of amino acid for different frequencies is simulated by Tanner EDA tool version 16.0 where we used 500 nm MOS technology and study their behaviour for characterization.

III. RESULTS AND DISCUSSION

All the simulations are done by S-Edit in tanner EDA tool. Each amino acid circuit is treated as an individual system and we simulated them within a range of (1 Hz-400 Hz) frequencies. The authors consider only the hydropathy index [10] value of the amino acids to characterize the amino acid as hydrophobic (water fearing amino acid) or hydrophilic (water loving amino acid). In Fig.2 [a-d] shows that the passive as well as corresponding active electrical model for one of the hydrophobic amino acid, Alanine along with the responses of the circuits. The circuits are excited by sinusoidal signal of 0.5V and frequency of 10 Hz. One of the hydrophilic amino acid , aspartic acid also presented here with its passive and active model in Figure 3 (a) and (b) respectively and excited by the same signal. The simulated waveforms for its passive and active circuit are depicted in Figure 3(c) and 3(d) respectively. It has been observed from simulated result in Figure 2 and 3, the range of amplitude response of hydrophobic amino acids are greater than 10mV and less than 10 mV for hydrophilic amino acids for a particular frequency (~10 Hz) and always amplitude response for hydrophobic amino acids greater than hydrophilic amino acids for different frequencies. The plots for the amplitude response of hydrophobic and hydrophilic amino acids are shown in Figure 4 and Figure 5 respectively. The amplitude response of the hydrophobic amino acids always more than hydrophilic amino acids which proves the hydropathy index value and the impedance of hydrophobic amino acids are higher than hydrophilic amino acids. It has been measured the power dissipation for the amino acids using MOS technology is 394.18 nW while power dissipation is 50 mW for its passive counterpart. The amino acids designed by MOS technology consume low power and it requires less space, so it can be useful for low power VLSI present trend.

IV. CONCLUSION

The electrical circuit model realization of amino acids and study their behaviour play a significant role in the present bioinformatics research. The amplitude response of the systems broadly classifies amino acids into two groups, hydrophilic and hydrophobic. This circuit model concept may help to detect particular genetic disease and also be useful in VLSI technology to develop electronic bio-sensing devices. It is increasingly important for engineers and scientist to process the biological data which is available in public domain [11] in a way that will be helpful for humankind.

ACKNOWLEDGMENT

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REFERENCES

[1] P. P. Vaidyanathan, “Genomics and proteomics: A signal processor’s tour”, IEEE Circuits Syst. Mag., vol. 4, no. 4, April 2004, pp. 6–29.
[2] R. Marshall, “Modeling DNA/RNA Strings Using Resistor–Capacitor (RC) Ladder Networks”, The Computer Journal, vol. 53 no. 6, 2010, pp. 644- 660.
[3] R. Marshall, “Modeling amino acid strings using electrical ladder circuits”, Nature & Biologically Inspired Computing., IEEE, Dec. 2009, pp. 1580-1583.
[4] G. Sampath, “RLC(M) circuit models of protein structure: analysis, visualization, shape synthesis, and pattern matching”, Proceedings of the 40th Conf. on Information Science and Systems (CISS 06), Princeton University, Princeton, NJ, USA, March 2006, pp. 1623-1628.
[5] R. Marshall, “Secondary structures and secondary structure linkages of protein sequences”, Systems Man and Cybernetics (SMC), IEEE, Oct. 2010, pp. 2995-3000.
[6] V. Hodzic, V. Hodzic, and R. W. Newcomb, “Modeling of the Electrical Conductivity of DNA”, IEEE Transactions on Circuits and Systems, vol. 54, no. 11, Nov. 2007.
[7] S. Mitra, S. Das, P. Pal Choudhuri, and S. Nandi, “Archtecture of a VLSI chip for modelling Amino acid sequence in Proteins”, 9th International Conference on VLSI Design, Jan. 1996.
[8] T. Roy and S. Barman, “Electrical Network Modeling of Amino Acid and its characterization”, IEMCON2013, ISBN: 978-81-923777-9-7.
[9] S. Barman, S. Saha, A. Mondal, and M. Roy, “Signal Processing Techniques for the Analysis of Human Genome Associated with Cancer Cells,” 2nd Annual international Conference IEMCON, Jan. 2011.
[10] J. Kyte, and R. F. Doolittle, “A simple method for displaying the hydropathic character of a protein,” J. Mol. Biol. 157, 1982, pp. 105–132.
[11] The NCBI website. [Online]. Available: http://www.ncbi.nlm.nih.gov/pubmed/15032603.

Schematic of Hydrohpobic Amino Acid

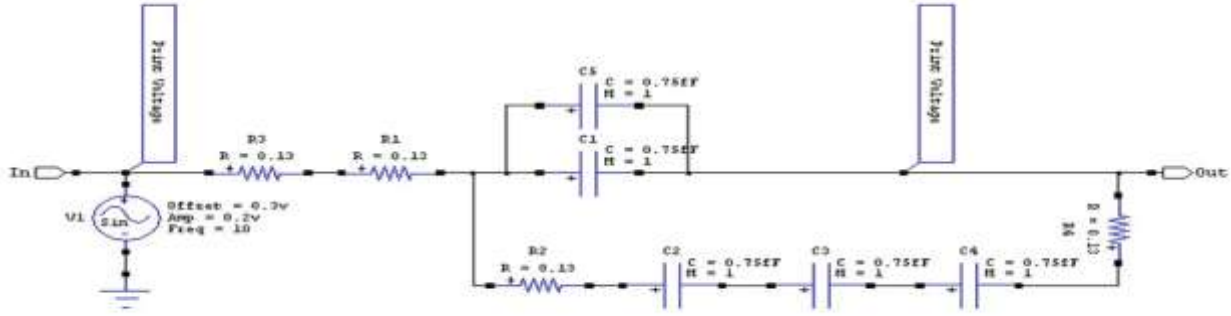


Fig. 2.(a): Realisation of amino acid (Alanine) Model Using Passive Component

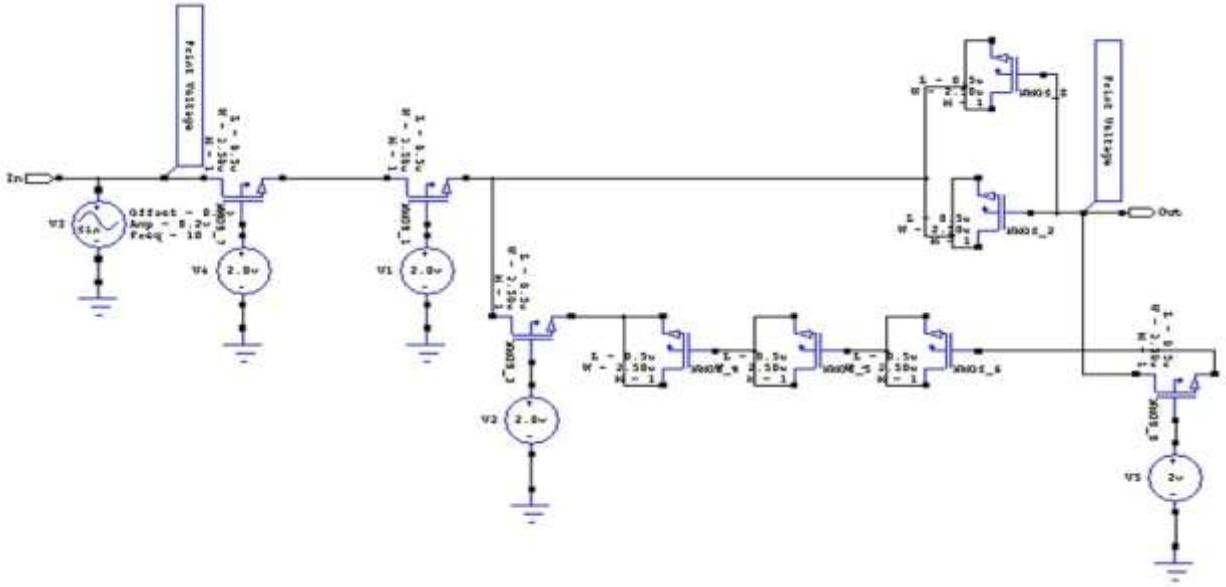


Fig. 2.(b): Realisation of amino acid (Alanine) Model using active MOS Component

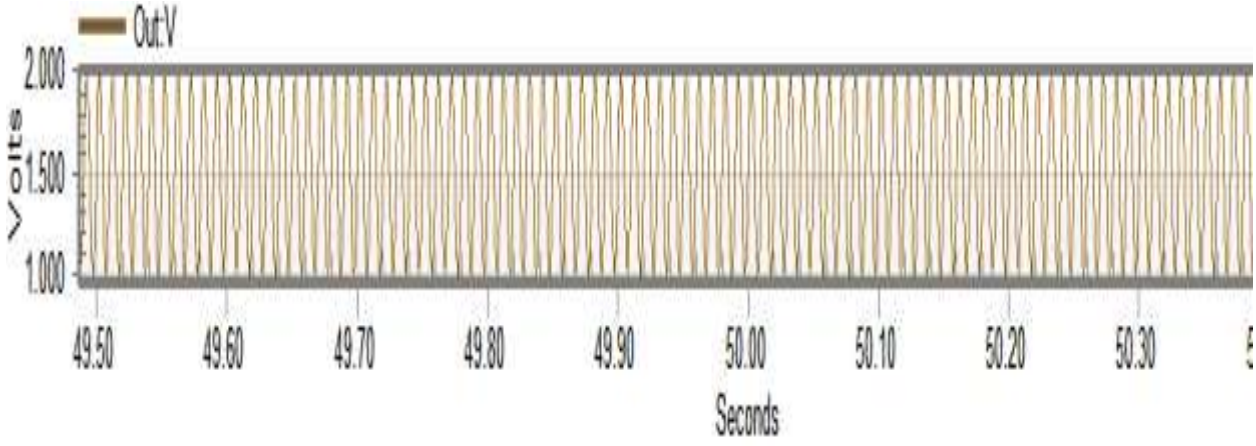


Fig. 2.(c): Waveform of amino acid (Alanine) using passive component

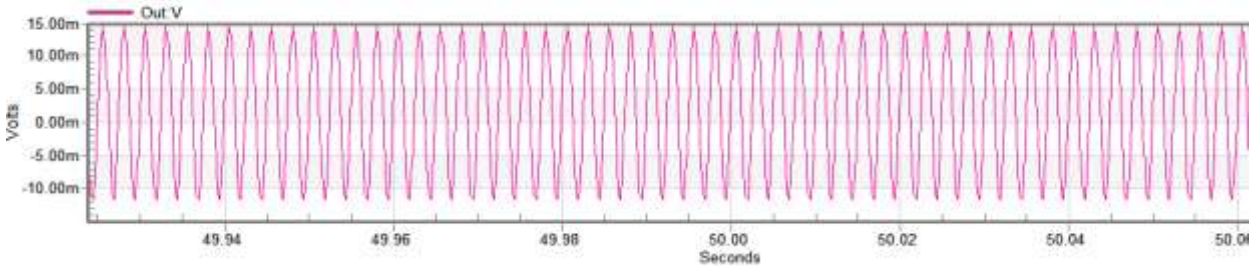


Fig. 2.(d): Waveform of amino acid (Alanine) using active MOS component

Schematic of Hydrophilic Amino Acid

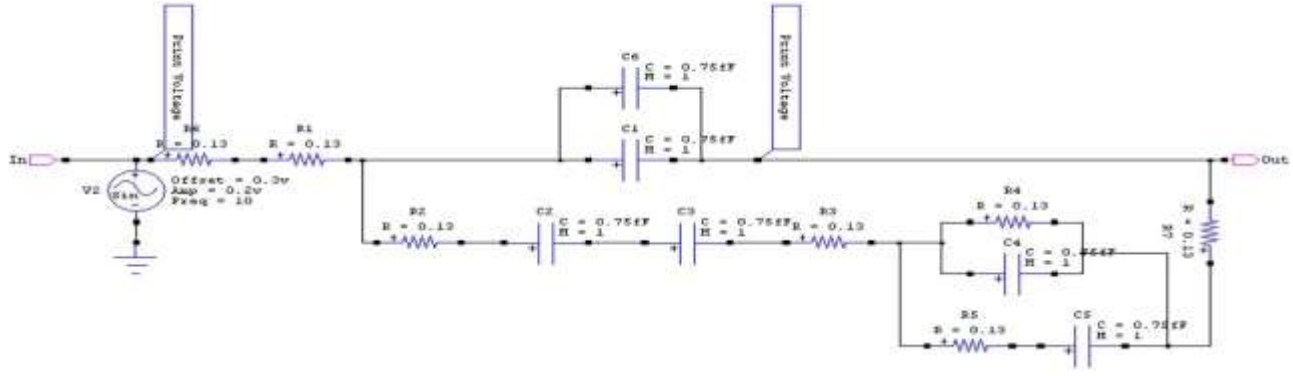


Fig. 3.(a): Realisation of amino acid (Aspartic Acid) Model using Passive Component

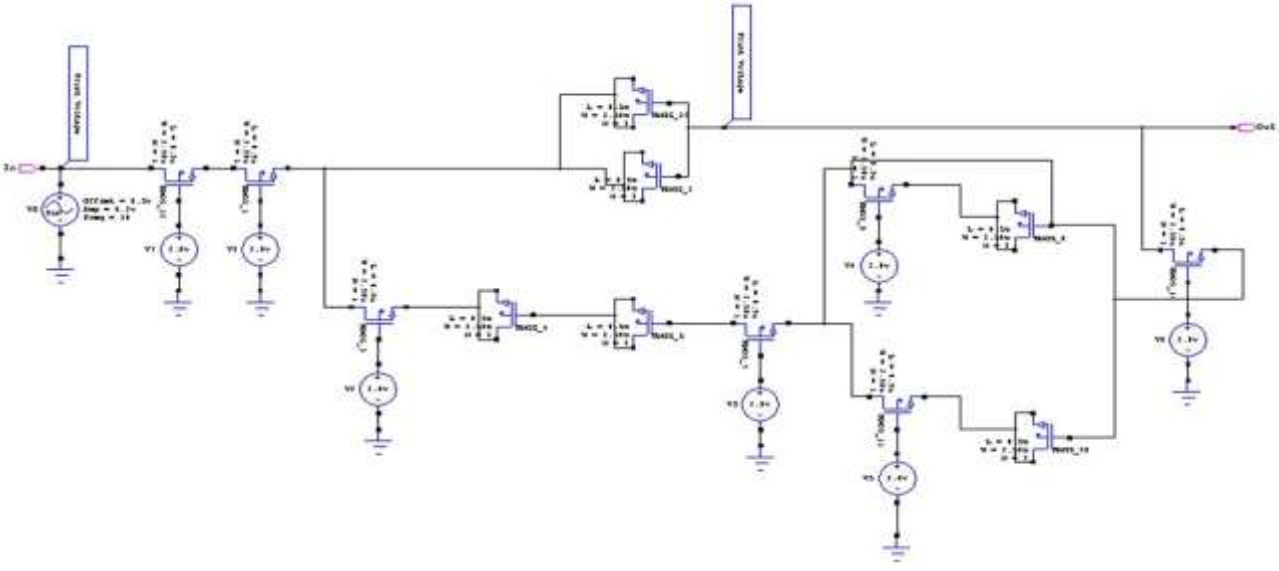


Fig. 3.(b): Realisation of amino acid (Aspartic Acid) Model using active MOS Component

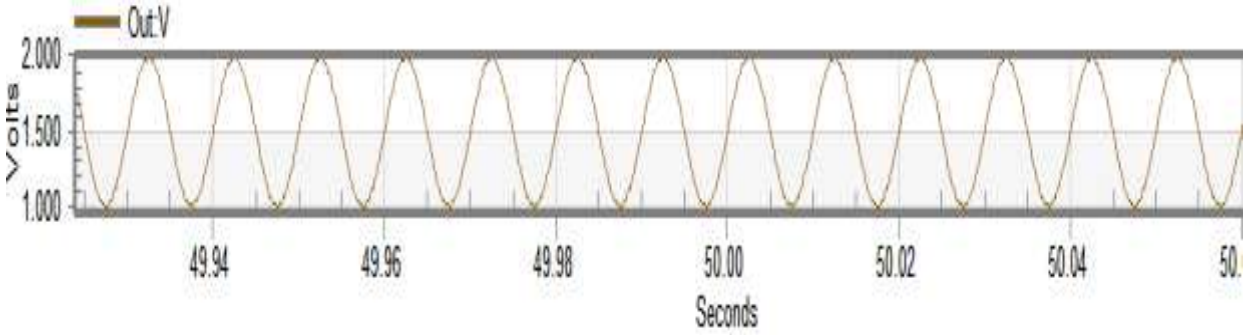


Fig. 3.(c): Waveform of amino acid (Aspartic Acid) using passive component

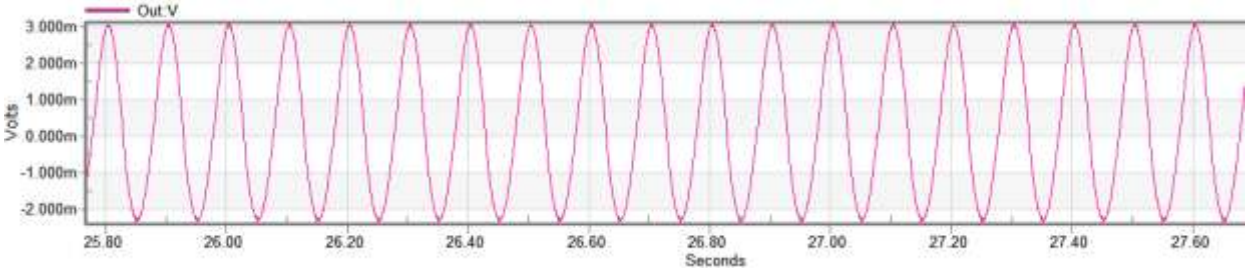


Fig. 3.(d): Waveform of amino acid (Aspartic Acid) using active MOS component

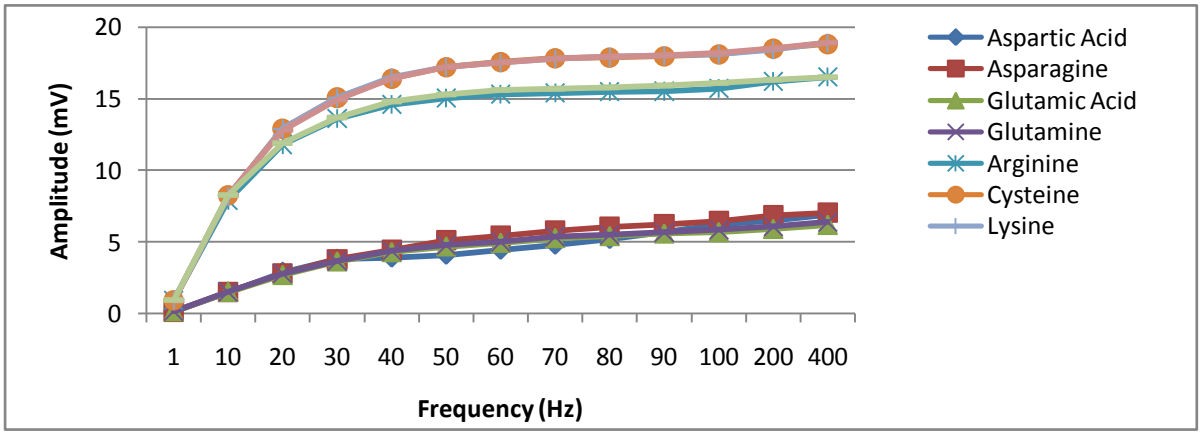


Fig. 4: Characteristics of Hydrophilic Amino Acids with frequency

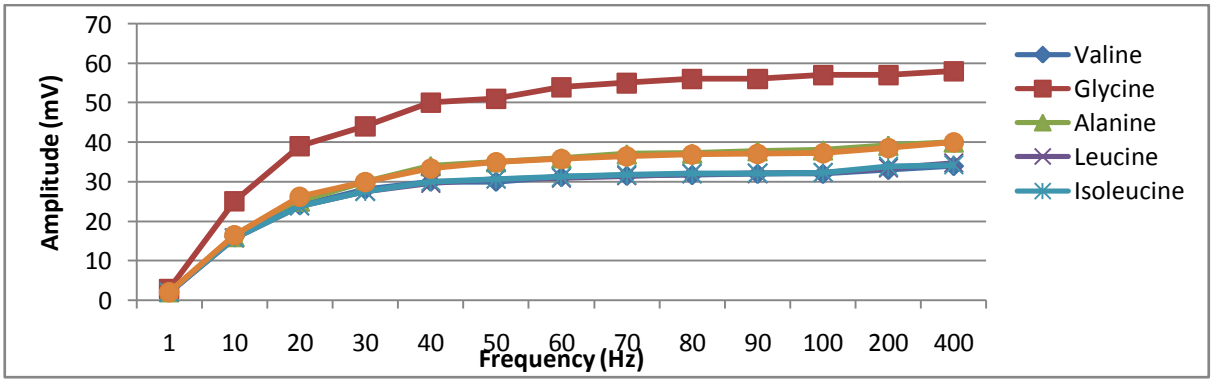
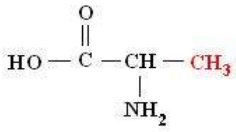
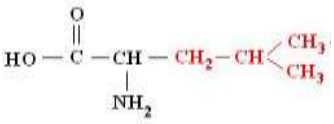
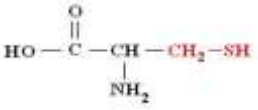
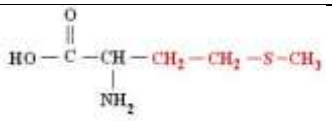
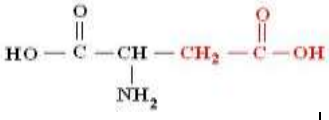
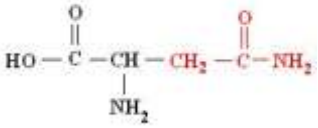
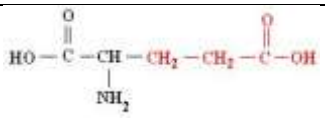
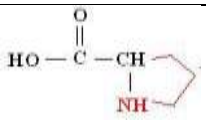
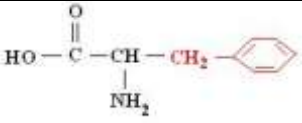
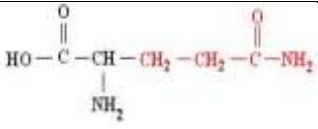
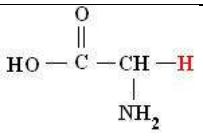
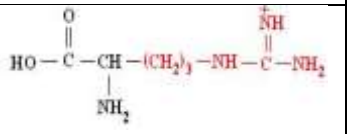
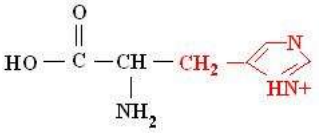
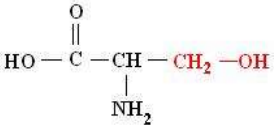
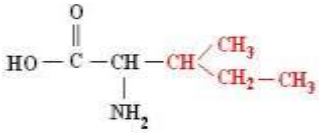
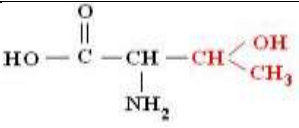
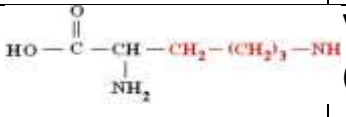
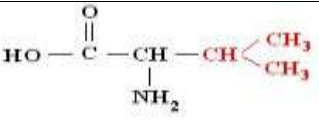
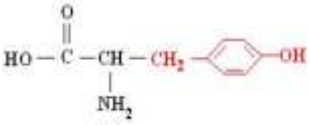


Fig. 5: Characteristics of Hydrophobic Amino Acids with frequency

TABLE 1: LIST OF AMINO ACIDS

Amino acids	Chemical structure of amino acid [side chain group (red)]	Amino acids	Chemical structure of amino acid [side chain group (red)]
Ala (A) **(Hydrophobic)**		**Leu (L)** **(Hydrophobic)**	
Cys (C) **(Hydrophilic)**		**Met (M)** **(Hydrophobic)**	
Asp (D) **(Hydrophilic)**		**Asn (N)** **(Hydrophilic)**	
Glu (E) **(Hydrophilic)**		**Pro (P)** **(Hydrophobic)**	
Phe (F) **(Hydrophobic)**		**Gln (Q)** **(Hydrophilic)**	
Gly (G) **(Hydrophobic)**		**Arg (R)** **(Hydrophilic)**	
His (H) **(Hydrophilic)**		**Ser (S)** **(Hydrophilic)**	
Ile (I) **(Hydrophobic)**		**Thr (T)** **(Hydrophilic)**	
Lys (K) **(Hydrophilic)**		**Val (V)** **(Hydrophobic)**	
Tyr (Y) **(Hydrophilic)**		**Trp (W)** **(Hydrophobic)**