

Letter to the Editor

Computer-Aided Pharmaco-Investigator: A Biomedical/Bioengineering Device for Pharmacological Investigations

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Pharmacological evaluations using clinical procedures have recorded huge consumption of resources (equipments, reagents, animal tissues, micro-organisms, viruses, etc), and time [1]. For example, a simple experiment like determination of Histaminic activity of a drug/extract may involve a simple apparatus like Kymogram [2]. This is not the same with an experiment that entails cardiovascular or brain examinations. They require sophisticated and expensive equipments [3]. An ileum of a guinea pig may be sufficient for a moderate pharmacological class experiment [2]. However, toxicological assessment of a drug/extract will attract the “sacrificing” of about 60 albino rats/guinea pigs [4]. Regarding time, a simple clinical laboratory-based microbial drug resistance assay takes 48 hours of incubation [5]. In a hospital setting, patients may have wait for such a long time before decisions are made regarding appropriate drugs of choice for their ailments. This is different in the case of computerized procedures. Assessments are achieved in seconds.

We have earlier proposed a biomedical/bioengineering device “Computer-Aided Pharmaco-Investigator” in a publication titled “Novel Computerized Approaches to Investigating Pharmacological Activities” [6]. The concept of the device is also highlighted in [7,8]. As shown in these studies, “Computer-Aided Pharmaco-Investigator” engages Sequence Information and Digital Signal Processing (DSP) Bioinformatics-based procedures such as Informational Spectrum Method (ISM) in order to help translate protein functions into numbers, which they further analyze so as to unearth the hidden bio-functionalities [9,10].

This procedure entails converting proteins (amino acids in sequences) engaged into sequences of number using the corresponding numerical values of the appropriate Molecular Descriptor/Biological Parameter. The values are obtained from the Amino Acid Index Table [11] such as deposited in the www.genome.jp/aaindex. The numerical sequences (also called signals) obtained as a result are then analyzed using Discrete Fourier Transform (DFT) [12]. The DSP method engaged in “Computer-Aided Pharmaco-Investigator” has preliminarily been detailed [6,9,10,13-17]. DSP procedure is the basis of technologies like Radar, Speech Detector, Image Processing, etc., [12]. “Computer-Aided Pharmaco-Investigator” is employable on all pharmacological agents, which are either protein/peptide-based or

have protein targets, or genes/protein encoding them. The sequence information obtained from these sources is known to carry as much biological information as the pharmacological agents [7,8].

The procedure engaged in the “Computer-Aided Pharmaco-Investigator” has assisted in developing other devices including Computer-Aided Drug Resistance Calculator (Patent Application filed in 2014) and Computer-Aided Vaccine Potency Assessor” (Inno Centive Winning Solver Award ID: 9933477). Cardio-protective effects of the Influenza vaccine [13] as well as comparison of the efficacies of drugs (Enfuvirtide and Sifuvirtide) and Plasmodial vaccine candidates Peptides P18 and P32 [14] have been studied using Computer-Aided Pharmaco-Investigator techniques. Other such investigations include the shield offered by Anthrax Protective Antigen [15], the amino acid sequences of Hepatitis C Virus that are responsible for the Interferon/Ribavirin therapeutic efficiency [16]. It has helped examine pharmacological properties of over 1000 agents including proteins from Influenza, Ebola, Anthrax, HIV and others, and proteins from functional groups like Tumor Necrosis Factors (TNF), Protease inhibitors, Heat Shock Proteins (HSP), Oncogenes, etc., [17]. Several bio-active drugs and vaccines as well as their candidates have been designed using the “Computer-Aided Pharmaco-Investigator” approach [17].

We have in a recent Research News Article demonstrated that “Pharmacists, Manufacturers of Pharmaceuticals, Clinicians, Scientists, Researchers and Environmentalists can now carry out their normal functions without engaging reagents and equipments but Computers only”. In line with these, we present a biomedical/bioengineering device to be named “Computer-Aided Pharmaco-Investigator” for use in pharmacological investigations in our various universities, research institutes, etc.

References

1. W.O.F.A.H. (OIE). Laboratory Methodologies for Bacterial Antimicrobial Susceptibility Test. 2008.
2. Yamasaki M, Matsumoto T, Fukuda S, Nakayama T, Nagaya H, Ashida Y. Involvement of thromboxane A2 and histamine in experimental allergic rhinitis of guinea pigs. *J Pharmacol Exp Ther.* 1997; 280: 1471-1479.
3. Groot A, Bots ML, Rutten FH, den Ruijter HM, Numans ME, Vaartjes I. Measurement of ECG abnormalities and cardiovascular risk classification: a cohort study of primary care patients in the Netherlands. *Br J Gen Pract.* 2015; 65: e1-8.
4. Korani M, Rezayat SM, Arbabi Bidgoli S. Sub-chronic Dermal Toxicity of Silver Nanoparticles in Guinea Pig: Special Emphasis to Heart, Bone and Kidney Toxicities. *Iran J Pharm Res.* 2013; 12: 511-519.
5. W.O.F.A.H. (OIE). OIE International Standards on Antimicrobial Resistance. 2008.
6. Nwankwo N, Molokwu G, Njoku N. Novel Computerized Approaches to Investigating Pharmacological Activities. *Computational Biology and Bioinformatics.* 2015; 3: 52-64.

7. Nwankwo N. Can Bio-functionalities be deciphered from Protein Sequence Information using Computational Approaches? 29th Annual Symposium of the Protein Society Book Abstract: 407. 2015.
8. Nwankwo N. Direct Computerized Translation of Biological data into Biological Information is now feasible: the Gains of Digital Signal Processing-based Bioinformatics Techniques. *Virol-mycol.* 2015, 4: 52.
9. Veljković V, Cosić I, Dimitrijević B, Lalović D. Is it possible to analyze DNA and protein sequences by the methods of digital signal processing? *IEEE Trans Biomed Eng.* 1985; 32: 337-341.
10. Veljkovic V, Veljkovic N. Characterization of conserved properties of hemagglutinin of h5n1 and human influenza viruses: possible consequences for therapy and infection control. *BMC Structural Biology.* 2009; 9: 1-11.
11. Tomii K, Kanehisa M. Analysis of amino acid indices and mutation matrices for sequence comparison and structure prediction of proteins. *Protein Eng.* 1996; 9: 27-36.
12. Smith SW. *The Scientist and Engineer's Guide to Digital Signal Processing.* California Technical Publishing. 2002.
13. Veljkovic V, Glisic S, Veljkovic N, Bojic T, Dietrich U, Perovic VR, et al. Influenza vaccine as prevention for cardiovascular diseases: possible molecular mechanism. *Vaccine.* 2014; 32: 6569-6575.
14. Nwankwo N. Signal processing-based Bioinformatics methods for characterization and identification of Bio-functionalities of proteins. De Montfort University. Leicester, United Kingdom. 2012.
15. Doliana R, Veljkovic V, Prljic J, Veljkovic N, De Lorenzo E, Mongiat M, et al. EMILINs interact with anthrax protective antigen and inhibit toxin action *in vitro.* *Matrix Biol.* 2008; 27: 96-106.
16. Veljkovic V, Glisic S, Veljkovic N, Jovanovic Cupic S, Prljic J, Gemovic B, et al. Assessment of Hepatitis C Virus protein sequences with regard to interferon/ribavirin combination therapy response in patients with HCV genotype 1b. *Vaccine I.* 2014; 32: 6569-6575.
17. Cosic I. Macromolecular bioactivity: is it resonant interaction between macromolecules?--Theory and applications. *IEEE Trans Biomed Eng.* 1994; 41: 1101-1114.