

Designing and Developing Therapeutic Interventions in the Bioinformatics Era

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Discovery, design and development of therapeutic interventions in this dispensation have traversed beyond serendipity [1]. The era of stumbling into active curative agents has been overtaken by the methodological and arduous processes involving laboratory-based investigations, clinical trials, and industrial formulation and production of drugs, vaccines and medical devices.

Laboratory-based clinical investigations involve identification, extraction and isolation of biologically active constituents [2]. This is followed by evaluation of pharmacological activities as well as standardization. Assessment of therapeutic indices (risk-benefit ratio), safety and applicability involve clinical trials, first on animals and then, human. If the therapeutic agent is approved, it is then mass produced depending on the scope of the users. Global ailments such as HIV/AIDS are expected to attract larger production than localized diseases like Malaria, which is a tropical illness. The entire process of discovery, design and development of therapeutic interventions is financial involving [2].

From the fore-going, it is evident that laboratory-based clinical investigations remain pivotal in the successful hunting of any therapeutic intervention. However, these investigations are found to be resource-consuming, expensive and time-wasting [3]. Since serendipity has eluded discovery and designing of therapies, clinical approaches are irrational, and computing knowledge as well as application of artificial intelligence have escalated [1], computer-assisted approaches and robotic devices have therefore crept into the processes of discovery, design and development of therapeutic interventions. The entire processes of hunting for therapies had transited into Computer-Aided Drug Design [4]. This approach to innovating therapies spans from the computer-assisted designing of drug molecules (Molecular Modeling) [5] and Structure-based Modifications [6] to the Absorption, Distribution, Metabolism and Excretion (ADME) [7] assessment and, the large-scale determination of the drug side effects that recently benefitted from the rationality of computation [8]. Other therapeutic interventions that would not have come out of serendipity are the trans-Atlantic surgery [9] and the machine-managed insulin delivery device for the diabetics [10].

As a result of these activities, there is currently, a large deposit of information needed for the discovery, design and development of therapeutic interventions. It has become too challenging to manage these information and therefore, an approach which would help retrieve, organize, analyze these huge data in order to extract, extrapolate, correlate, juxtapose, reconcile and predict outcomes is required. This has brought in Bioinformatics approaches into the invention of therapeutic interventions, which is the only technique that can perform these functions [11].

Bioinformatics tools and programs are bound for these purposes. These devices encompass apparatuses for the search for drug molecules, designing and determination of their potency, resistance and unwarranted effects. The devices involved in the search include High-Throughput Screening (HTS) [12]. Designing involves two

approaches. They are Molecular Modelling [5], which includes Docking [13] and Structure-based optimization [14], where analysis such as Multiple Sequence Alignment [15] and Digital Signal Processing-based [16] are undertaken. Drug resistance algorithms such as Genotype, Phenotype and a combination of both including Virtual Phenotype are Bioinformatics-based.

This journal tends to explore these Bioinformatics techniques that evolved from the Botanic age where herbalists are the bone setters and healers, the all-knowing in therapy.

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Received August 17, 2012; Accepted August 18, 2012; Published August 20, 2012

Citation: Nwankwo N (2013) Designing and Developing Therapeutic Interventions in the Bioinformatics Era. Drug Des 2: e107. doi:[10.4172/2169-0138.1000e107](https://doi.org/10.4172/2169-0138.1000e107)

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