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Mini Review

Artificial Intelligence and Disease-Site Specific Targeting of Drugs

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Abstract

There has been much enthusiasm generated about possible application of Artificial Intelligence (AI) in biology and medicine. While "machine learning" facilitates to process huge data sets, its effective use to parallel human creative thinking including perception, abstraction, memory, imagination and intuition is not yet an option. Application of such advanced AI will be needed to solve complex tasks such as disease-site specific targeting of therapeutic agents.

Keywords: Disease-Specific; Drug; Targeting; Artificial Intelligence

The amount of medical knowledge is increasing at an exponential rate. Effort it takes to read and keep up with this amount of new information has become excessive for medical professionals and researchers. The time has come to consider the use of Artificial Intelligence as a necessary tool to process knowledge resources and move forward in an informed and rational manner.

The possibility of delivering drugs to site of diseases without causing off-site undesirable effects has been considered for more than a century but effective targeted drug delivery has not been realized. Numerous publications continue to appear that promise to "deliver" but fail to enable generation of therapeutic products [1-3].

Apart from our still incomplete understanding of diseases, one of the main reasons for these failures is that researchers do not recognize, or choose to ignore what is needed. Using a recent publication as an example, composite particulates with targeting, chemotherapeutic, and magnetothermal functionalities were suggested to have therapeutic potential in treating breast cancer [4]. The publication presented fine work in the area of material science, however its conclusion based solely on data showing killing of breast cancer cells in vitro is nothing more than speculation.

Developers of targeted drug-delivery system must be fully aware and consider the pharmacokinetic requirements that need to be fulfilled for deriving benefit from site-targeted delivery. Research has clearly established the essential requirements that need to be met [5-8]. Further, it has been argued that there is an essential need to identify unique molecular targets of disease [9].

Traditionally, serendipity is considered an important factor in finding new drugs. Random testing has generated new drug candidates so has some merit, however its rate of success is low. On an average, random-testing assays typically identify not more than 3% of the tested compounds as drug candidates showing properties that may warrant further laboratory and animal testing. Going forward, only about ten of these qualify for testing in humans [10]. It has been suggested that "Careful decision-making during drug development is essential to avoid costly failures" [11]. An idealistic and facetious suggestion that one needs only one chemical entity to develop a new drug as long as one makes only correct decisions during the process is not achievable in practical drug development.

The latest estimate puts the cost of developing one new drug at $2.6 billion, with the rate for new chemical entities (NCE) to become approved drugs being less than 12% [12]. In early 2019, FDA approved a gene therapy drug costing $2.1 million for one-time treatment for spinal muscular atrophy. This introduces a new type of medicine – a drug that can cure patients in a single treatment. It poses a challenging question to be answered: "Is any drug worth millions of dollars, even if it saves lives?" [13].

Given the above challenges, Artificial Intelligence will need to be employed to utilize existing experience and generate "intelligent"

approaches to creating and testing new drugs to minimize failures. Several pharmaceutical companies have now started to use a form of AI – "machine learning" [14]. However, there is much skepticism about the likelihood of success given the length and complexity of drug development, and a high rate of drug candidates' failure. It has been proposed that there is an opportunity to change the conventional drug development through implementing collaborations between universities, governments, and the pharmaceutical industry to optimize resources [15]. However, the practice and need to maintain proprietary secrets will likely stand in the way of a broad and effective collaborations. Recent report by Buvailo and Ajami [16] reviewing research trends in biopharmaceutical industry included rapidly growing use of AI in drug discovery and development, applied to tasks such as "mining" of data, target identification, and divining properties and risks of new drug candidates. AI has been able to assist with data-rich areas such as designing chemical syntheses, planning complex activities such as pre-clinical and clinical research and in evaluating resulting data. While AI is being applied in matching drugs to existing targets, it is clear that identifying molecular structures uniquely associated with diseases continues to be an unmet need [17], recognizing that claims made about AI may be "overhyped".

To a large extent, finding and developing new chemical entities into drugs is a "groping in the dark" activity. For example, a recent publication reported that "Macrocycles are unlikely yet potent drugs" [18]. The authors speculated that a special property of often extremely large (above 800 Da) natural macrocycles passively to diffuse through cell membranes is due to their ability to reorganize their conformation depending on the vehicle. They synthesized over one million macrocycles that include structural elements often found in natural biologically active macrocycles. Developing these compounds into therapeutically useful entities using the current drug-development processes will be a mammoth task without having additional relevant information about their properties and diseases. A positive major step forward could be made by adopting a more rational approach based on understanding of what drives diseases at the molecular level, and in particular what unique molecular structures are involved that are not shared by non-disease cells. This approach has been very effective for curing bacterial and recently even viral infections in which molecular features of organisms foreign to human body were identified. When applied to other diseases, such knowledge would enable development of truly disease-targeted drugs. To this end, it is very likely that Artificial Intelligence will need to be employed [19].

Machine learning - the capability to process large amounts of data – is typically the first thing one thinks when AI is mentioned. With AI, the tasks of extracting information from thousands or more data points become very facile. Further, the current AI is at a level that it can understand natural language and is even capable of limited, basic interactions with humans (such as Siri).

Application of AI to finding molecular basis of disease will, however, require full human-level intelligence. It will require for the AI to assimilate all the existing data on the topic, all the current assumptions and theories about how disease originates and progresses, and how it could be cured. It will need to go beyond extracting information, and draw novel conclusions and recommendations on what steps need to be taken to reach the ultimate goal – understanding the disease and defining unique molecular structures. It will need to foresee ways of making use of this information. To this end, it will need to be fully competent in intelligence of the given topic. In other words, it will need to acquire full capabilities in all aspects of human intelligence such as being able to perceive the real world beyond the information given to it by its programmers. It will need to have the ability to determine the significance of various parts of the overall task and decide on which to focus. It will need to acquire the manner of processing information in human-thinking terms such as perception, abstraction and memories, apply critical analysis of the information and then remember and recall outcomes as and when needed to synthesize a new, more complex whole. Ultimately, it will need to have the capacity to generate new knowledge and know-how. Will AI be able to speculate and imagine? It will need to. Will it be able to reason? It will have to. Will it be logical where humans often cannot be? Will it be able to handle the "what if" questions and predict, and make decisions? All that and more. It would better be. But very likely an intelligent input from humans will be needed all along the way to solve this challenging task at hand.

Conclusion

Given the complexity of disease-related biology and of the process of developing effective human therapies, it is paramount that Artificial Intelligence is applied effectively to analyze all the available data on the road to making right decisions. However, an intelligent input from humans will need to be continued to solve challenging tasks such as disease-specific targeting of drugs.

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