Chapter 19
Cancer Precision Drug Discovery Using Big Data and Artificial Intelligence Technologies

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ABSTRACT

Improved cancer treatments are widely cited as a significant unmet medical need. Recent technological developments and the increasing availability of biological "big data" provide an unprecedented opportunity to systematically classify the primary genes and pathways involved in tumorigenesis. Artificial intelligence (AI) has shown great promise in many healthcare fields, including science and chemical discovery. The AI will explore and learn more using vast volumes of aggregated data, converting this data into "usable" information. The aim is to use current computational biology and machine learning systems to predict molecular behaviour and the probability of receiving a helpful medication, thus saving time and money on unnecessary tests. Clinical trials, electronic medical records, high-resolution medical images, and genomic profiles can all be used to help with drug growth. The discoveries made with these emerging technologies have the potential to lead to innovative therapeutic approaches.

1. INTRODUCTION

Cancer is a significant and growing global health burden, accounting for over 12 million newly diagnosed cases each year and more than 15% global deaths. The development of new, improved cancer therapies is frequently mentioned as an unmet medical need (Varmus & Kumar, 2013). Cytotoxic agents have traditionally dominated cancer therapies. These therapies, which cause DNA damage that exceeds a

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cancer cell's ability to repair itself, have been a mainstay of cancer chemotherapy for more than 30 years (Pearl et al., 2015). Although these agents effectively treat testicular and breast cancers and childhood leukaemias, they are relatively ineffective in treating many cancers, including lung, brain, pancreatic and esophageal tumors, even when used in combination (Mukherjee, 2011; Varmus, 2006). Recently, the emphasis on drug discovery has shifted to identifying genomic and other molecular abnormalities in cancer subtypes to develop targeted therapies with the potential for greater efficacy and therapeutic selectivity (Yap & Workman, 2012). Early success stories of single-agent targeted therapies appeared to be very promising. Trastuzumab (Garnock-Jones et al., 2010) and imatinib (Stagno et al., 2016) are two critical examples used to treat breast cancer and chronic myeloid leukemia, respectively. Trastuzumab is a monoclonal antibody targeting cells overexpressing the human epidermal growth factor receptor HER2/ERBB2, whereas imatinib, a small molecule, inhibits constitutively activated Abl kinase caused by the BCR-ABL translocation. While some of these targeted therapies have been particularly effective, it appears that they are somewhat unusual, as some of the newer targeted therapies have only provided brief remissions before resistance develops (Al-Lazikani et al., 2012; Garraway & Jänne, 2012).

On the other hand, recent advancements in technologies have provided an unprecedented opportunity to comprehensively identify the alterations, genes, and pathways involved in tumorigenesis, raising the prospect of extending targeted therapies (Garraway & Lander, 2013; Stratton, 2011). Many innovative approaches and technologies have been implemented in drug discovery over the last 25 years. Next-generation sequencing and large-scale RNAi interference and, more recently, CRISPR technology have proven helpful for mechanistic biological exploration and drug target identification, particularly in oncology. The size and diversity of chemical libraries have grown. Also, the high-throughput screening has increased the availability of chemical matter acting on drug targets, while the structure and fragment-based design has improved hit-to-lead and optimisation of small molecules. Recombinant DNA technology has revolutionised the design of therapeutic antibodies, and around the same time, the drug discovery ecosystem has become more dynamic. Academic drug development and chemical biology are expanding in scope, as it is open innovation, and various forms of collaborations involving academia and the pharmaceutical and biotechnology sectors are now widespread (Varmus & Kumar, 2013). These modifications increase creativity and help to spread the risks of drug development. Mechanism-driven drug development is now the standard, owing to unparalleled knowledge of disease's molecular basis. Oncology has had the most groundbreaking first-in-class drug approvals (Pearl et al., 2015). The discovery of pathogenic molecular mechanisms supports this, most recently through the genome sequencing of tens of thousands of cancer patients, ushering in the era of precision medicine in oncology (Varmus, 2006). As a result, many genetically targeted medications can now be provided to cancer patients based on their risk level. These targeted drugs frequently target a specific addiction or vulnerability in the tumor identified using a predictive molecular biomarker included in the drug label (Mukherjee, 2011; Yap & Workman, 2012). The new generation is also making a significant impact on immuno-oncology drugs.

Meanwhile, the Big Data revolution has an increasing impact across multiple domains, affecting many aspects of our daily lives and numerous areas of research (Stagno et al., 2016). This is due to the increased availability and lower costs of technologies for generating, storing, and analysing large and diverse data sets. Some aspects of multidisciplinary drug discovery, particularly medicinal chemistry, have long embraced computational methods and the collection and analysis of Big Data to aid decision-making (Garraway & Jänne, 2012). The mining of raw biological data on a large scale for target hypotheses is now commonplace. Despite advancement, the drug discovery community is still a long way from understanding the full potential of Big Data analytics and Artificial Intelligence (AI). In this article, we