Natural Products for Anti-Cancer Progress: The Impact of Artificial Intelligence †

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Abstract: Finding for more effective anticancer drugs on almost different types of cancer, a huge number of molecules is still under evaluation and barely many more than 100,000 compounds have been tested with researchers and several institutions since recent decades. The fact that plant-derived molecules are treated at various levels against cancer is based on a very long history. This has enabled many molecules derived from plant sources to be used in cancer treatment. With the introduction of artificial intelligence, studies on the discovery of new molecules that may be effective in the etiology of various diseases have gained weight as in every field. Artificial intelligence learns the relationship between molecular structure and biological components in certain mathematical algorithms with the obtained *in vitro* and *in vivo* values and helps to create new molecular patterns as a result of certain validations. In fact, the artificial intelligence, is now able to develop novel algorithms over the initially defined and further realization might proceed new designs with advanced programming by self-settings new routes through the improvement of desired targets. The introduction of the genetic profile and consequently the discovery of new drug molecules will be one of the most important fields of study of the future. Molecules to be obtained from plant sources will also have very important roles in this direction. Drug therapy for patients with the same disease but with a different genetic profile does not give the same treatment success in every patient. The reason for this is that due to the different mutations in DNA, the protein structures encoded by the genes show differences and the interaction pattern of molecules on the proteins responsible for diseases, could be different. Therefore, for each patient, due to the mutation, diverse molecules that can interact with mutated proteins should be required. This issue is becoming increasingly important all over the world, especially under the name of precision medicine and in the form of personalized drug administration, and demonstrates the importance of drug treatment depending on the individual's genetic profile. It is then useful to treat anticancer molecules of plant origin in this direction. For this purpose, gene rearrangements and gene editing procedures can be applied in plants by using CRISPR technology to improve several factors through leading to design and develop new plant origin molecules for the intended purpose with the assistance of artificial intelligence algorithms.

Keywords: artificial intelligence; plant-origin anti-cancer molecules; precision medicine; personalized drug therapy; genetic profiles; CRISPR