



Drug Discovery: A Non-Expiring Process

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Received: 22 April 2020 / Accepted: 22 April 2020 / Published Online: 22 April 2020

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Drug is "a substance used as a medication or in the preparation of medication" [1]. So many natural and synthetic chemical compounds have been examined to be qualified with this criterion for year; however, not all of the efforts have been successful for the purpose. From traditional medicine by prescribing natural resources for medications till today pharmaceutical industry based prescriptions, helping the patients to reorganize their injured life to normal life has been the major goal of drug discovery. There are many phases to reach a drug from millions of available chemical compounds, in which knowledge about the structural features of small molecule drug is necessary in addition to knowing the main cause of a disease [2]. Structure-Based (SB) and Ligand-Based (LB) drug discovery are two processes focusing on discovering a drug for a known cause of diseases in the former one (SB) and characterizing structural features of a small molecule to be qualified as drug in the latter one (LB) [3]. In this case various methodologies have been developed for the purpose such as synthesis in chemistry labs, biological examining *in vitro*, animal testing *in vivo*, up to human clinical trials evaluations. It is obvious that so much detailed information are inside each of mentioned methodologies, some known and some still unknown, in addition to human efforts and

spending time and money costs for years to reach a drug. To save overall human, equipment, time and money costs, novel methodology of drug discovery has been initiated *in silico* [4, 5]. The new media depends on theoretical foundation, mathematical algorithm, biological information, and silicon-based computation in the Central Processing Unit (CPU) of computers. Why should do this? Because we do not have so much time for years to discover a drug for a pandemic disease like COVID-19. Therefore, *in silico* drug discovery is considered as an emerging methodology to find a new drug with more details in shorter time, lower cost, and higher efficacy [6-11]. After this process is done, each of chemical synthesis, *in vitro*, *in vivo*, and clinical trials could be accelerated for confirmation of the arisen idea from *in silico* media. Despite the pandemic diseases, the patients involved with other ones such as cancer and even mood disorders do not have a clear prescription yet. Although the life is very much easier and comfortable in the improved industrial world, but genetic mutations are also very much common in this life style discarding the desired comfort. To this point, new diseases such as cancer and pandemic influenza or more significant effects of old diseases such as heart attacks in addition to mood disorders of machinery life are always arisen with more numbers of people

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requiring more efficient pharmacotherapies [12-15]. Moreover, the precision medicine is trying to personalize the specific therapy of disease for

each person as a new challenge of drug discovery. Therefore, it seems that there is no expiring for drug discovery.

References

1. Retrieved April 22, 2020, from <http://www.merriam-webster.com/dictionary/drug>.
2. Hill RG. Drug discovery and development-E-book: technology in transition. Elsevier Health Sciences; 2012.
3. Moro S, Bacilieri M, Deflorian F. Combining ligand-based and structure-based drug design in the virtual screening arena. *Expert Opin. Drug Discov.* 2007;2:37-49.
4. Rifaioğlu AS, Atas H, Martin MJ, Cetin-Atalay R, Atalay V, Doğan T. Recent applications of deep learning and machine intelligence on in silico drug discovery. *Brief. Bioinform.* 2019;20:1878-1912.
5. Mirzaei M. Science and engineering in silico. *Adv. J. Sci. Eng.* 2020;1:1-2.
6. Mirzaei M, Harismah K, Da'i M, Salarrezaei E, Roshandel Z. Screening efficacy of available HIV protease inhibitors on COVID-19 protease. *J. Mil. Med.* 2020;22:100-107.
7. Soleimani M, Mirzaei M, Mofid MR, Khodarahmi G, Rahimpour SF. Lactoperoxidase inhibition by tautomeric propylthiouracils. *Asian J. Green Chem.* 2020;4:1-10.
8. Nazemi H, Mirzaei M, Jafari E. Antidepressant activity of curcumin by monoamine oxidase-A inhibition. *J. Adv. Chem. B.* 2019;1:3-9.
9. Soleimani M, Mirzaei M. In silico pharmacy: from computations to clinics. *J. Pharm. Care* 2017;5:1.
10. Naderi E, Mirzaei M, Saghale L, Khodarahmi G, Gulseren O. Relaxations of methylpyridinone tautomers at the C60 surfaces: DFT studies. *Int. J. Nano Dimen.* 2017;8:124-131.
11. Harismah K, Sadeghi M, Baniyasi R, Mirzaei M. Adsorption of vitamin C on a fullerene surface: DFT studies. *J. Nanoanalys.* 2017;4:1-7.
12. Mirzaei M. Effects of carbon nanotubes on properties of the fluorouracil anticancer drug: DFT studies of a CNT-fluorouracil compound. *Int. J. Nano Dimen.* 2013;3:175-179.
13. Mirzaei M, Yousefi M. Computational studies of the purine-functionalized graphene sheets. *Superlat. Microstruct.* 2012;52:612-617.
14. Zare A, Mirzaei M, Rostami M, Jafari E. Photosensitization of phthalocyanine for singlet oxygen generation in photodynamic therapy applications. *J. Med. Chem. Sci.* 2020;3:55-59.
15. Samadi Z, Mirzaei M, Hadipour NL, Khorami SA. Density functional calculations of oxygen, nitrogen and hydrogen electric field gradient and chemical shielding tensors to study hydrogen bonding properties of peptide group (OC-NH) in crystalline acetamide. *J. Mol. Graph. Model.* 2008;26:977-981.

How to cite this article: Mirzaei M. Drug Discovery: A Non-Expiring Process. *Adv. J. Chem. B.* 2020;2(2):46-47. doi: [10.33945/SAMI/AJCB.2020.2.1](https://doi.org/10.33945/SAMI/AJCB.2020.2.1)