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Editorial

Lab-in-Silico Insights

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Recent developments in computer hardware and software, in addition to modern algorithms, have led to new era of scientific laboratories; called Lab-in-Silico. The simulation protocols have been evaluated for several types of chemical matters and reactions to simulate the real systems in the computers. There is no doubt in the importance of efforts in the experimental chemical laboratories to yield novel materials, but the simulation processes could push ideas into products at the higher accuracy. Knowledge about what happens during the reactions and the corresponding mechanisms is always an important task for those scientists working on the mystery of chemistry. Trial/error is one of the proposed solutions for this problem, but it is very much expensive in time and money without reliable efficacy in most cases [1]. In contrast, Lab-in-Silico provides high performance facilities to explore details of chemical reactions and mechanisms at the highest accuracy levels according to the approved theories and the available experimental data banks [2]. Various aspects of computational sciences including chemistry, physics, biology, mathematics and also engineering have been developed to achieve details of complicated scientific systems. Moreover, computer-aided drug design (CADD) has been developed based on the already developed computational aspects to bring medicinal ideas and problems from in vitro and in vivo laboratories to Lab-in-Silico [3]. Prior to the experimental effort or in parallel with it, the ideas could be very well examined or modified based on the computational approaches. Moreover, the characteristics of complicated systems could be very well recognized by the mentioned approaches. Classical and modern physics yielded quantum approaches to study several pointes of matters including structural features, reactivity potencies, spectroscopic properties and so many other aspects regarding the types of materials and required investigating methods. Intermolecular interactions, which are not fully recognized by the experimental laboratories, could be very well recognized by Lab-in-Silico [4]. In this case, important information about ligand-receptor interactions in novel drug design could be very well identified by the CADD protocols of Lab-in-Silico to make the best structural modifications in order to obtain the best ligand for the pharmacotherapeutic cares [5]. To this aim, several attempts have been done to learn about details of biological systems to propose the best candidates for further studies in experimental laboratories avoiding loss of time and money [6-11]. Hereby, Lab-in-Silico could assist the scientist

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to approve their ideas prior to any trial/error efforts of the experimental laboratories or in parallel with it to make a clear description of the obtained results.

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