Lab-in-Silico
https://lab-in-silico.com
eISSN: 2717-1922

EDITORIAL

Lab-in-Silico. 2020;1(2):31-32. DOI: 10.22034/labinsilico20012031

Making Sense the Ideas *In Silico*

Mahmoud Mirzaei✉

Biosensor Research Center, School of Advanced Technologies in Medicine, Isfahan University of Medical Sciences, Isfahan, Iran

Received: 28 December 2020 / *Accepted*: 29 December 2020 / *Published Online*: 30 December 2020

Improvements of computers hardware and software equipments have led to friendly using of these complicated systems especially in two last decades. Moreover, several types of mathematical algorithms, physical theories and chemical and biochemical concepts have been included in the computer systems. According to definition by Merriam-Webster, computer is "*a programmable usually electronic device that can store, retrieve, and process data*".[1] Therefore, if somebody wants to imagine by programing her/his mind, She/He could also do such parallel programming in the computer systems. In addition to local computers, Internet made possible using web-based computer systems very much farther from the user. So, a very good and powerful facility is available to make sense ideas of science and engineering.[2] Life science includes atoms of chemical species, rational relations of biological concepts, and reasonable concepts of physics, to make ordered life system. Chemistry, biology and physics are those fields of natural science, in which the ideas arisen from these categories could make a significant change for life science. Mathematics is somehow the binding bridge of all three fields and it could help to make algorithms to reach the goals more successfully. Indeed, computers for natural scientists are those programming electronic devices following the initial programming of mind. As a result, several ideas could be very well developed using the computer systems *in silico*.[3] However, using such process is almost a multi-factorial pattern from initiating the idea and developing it in computer.

Within two last decades, researches have paid considerable attentions to perform computer-based works in order to either predict or interpret experimental achievements.[4-6] Yes, this is true that the correlation between computational and experimental results is not 100 %, but the atomic-scale computations could yield such information not available in experiments.[7-10] Therefore, each of computational and experimental works has its own mission to explore its specific goal in the mysterious science and engineering world. Based on such importance, different branches of computer-based works have been developed such as Computational Chemistry, Computational Biology, Computational Physics, and so many other types of computations. Regarding such disciplines, several works have been reported in literature in both of single-standing disciplinary or multi-disciplinary of computations. Computer-Aided Drug Design is an example of a multi-disciplinary of computations using various elements to achieve the purpose.[11] Parallel to such developments, new journals have been also established to publish special works *in silico*.[12] Referring again to Merriam-Webster, "*in or on a computer : done or produced by using computer software or simulation*" is a definition for *in silico*.[13] Here it is very clear that the ideas could be very well initiated in mind and then they could be made sense *in silico* using local or web-based computer systems.[14-17] Let's try the science and engineering *in silico* after imagining them in mind to achieve significant goals as much as possible.

✉ Corresponding author; *E-mail address*: mdmirzaei@pharm.mui.ac.ir (M. Mirzaei).

REFERENCES

1. Merriam-Webster Dictionary. https://www.merriam-webster.com/dictionary/computer
2. Mirzaei M. Science and engineering *in silico*. Adv J Sci Eng. 2020;1:1-2.
3. Mirzaei M. Lab-in-Silico insights. Adv J Chem B. 2020;2:1-2.
4. Ozkendir O, Gunaydin S, Mirzaei M. Electronic structure study of the $LiBC_3$ borocarbide graphene material. Adv J Chem B. 2019;1:37-41.
5. Harismah K, Ozkendir OM, Mirzaei M. Lithium adsorption at the C_{20} fullerene-like cage: DFT approach. Adv J Sci Eng. 2020;1:74-79.
6. Ozkendir OM. Electronic structure study of Sn-substituted InP semiconductor. Adv J Sci Eng. 2020;1:7-11.
7. Mirzaei M. A computational NMR study of boron phosphide nanotubes. Z Naturforsch A. 2010;65:844-848.
8. Nouri A, Mirzaei M. DFT calculations of B-11 and N-15 NMR parameters in BN nanocone. J Mol Struct THEOCHEM. 2009;913:207-209.
9. Partovi T, Mirzaei M, Hadipour NL. The C–H···O hydrogen bonding effects on the 17O electric field gradient and chemical shielding tensors in crystalline 1-methyluracil: A DFT study. Z Naturforsch A. 2006;61:383-388.
10. Mirzaei M. The NMR parameters of the SiC-doped BN nanotubes: a DFT study. Physica E. 2010;42:1954-1957.
11. Soleimani M, Mirzaei M. *In silico* pharmacy: from computations to clinics. J Pharm Care. 2017;5:1.
12. Mirzaei M. Lab-in-Silico: An international journal. Lab-in-Silico. 2020;1:1-2.
13. Merriam-Webster Dictionary. https://www.merriam-webster.com/dictionary/in%20silico
14. Faramarzi R, Falahati M, Mirzaei M. Interactions of fluorouracil by CNT and BNNT: DFT analyses. Adv J Sci Eng. 2020;1:62-66.
15. 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.
16. Yaghoobi R, Mirzaei M. Computational analyses of cytidine and aza-cytidine molecular structures. Lab-in-Silico. 2020;1:21-26.
17. Tahmasebi E, Shakerzadeh E. Potential application of B_{40} fullerene as an innovative anode material for Ca-ion batteries: *In silico* investigation. Lab-in-Silico. 2020;1:16-20.

How to Cite: Mirzaei M. Making Sense the Ideas *In Silico*. Lab-in-Silico. 2020;1(2):31-32.
DOI: https://doi.org/10.22034/labinsilico20012031
URL: https://sciengpub.com/lab-in-silico/article/view/labinsilico20012031