Editor's Note

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Cheminformatics to Prompt the Process of Drug Discovery

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Chemical Informatics is one of the most emerging fields that add cutting edge state of information to the science. Its multidimensional approach is widely applied to discover and rediscover the drugs. This technology facilitates the minimizing of *in vivo* experimental period. It is a vast field that aims to disseminate information regarding the design, structures, creation, dissemination, visualization and the use of knowledge related to topics on Chemical information, Software and databases, Molecular modeling, Computer aided drug design, Molecular graphics, Data mining techniques etc,. The current Volume No 2, Issue 1, had published 3 research articles of current interest.

Researcher Noorbatcha's article tried to elaborate the role of structural features of seconucleosides for their anticancer activity. This study had constructed the quantitative structure activity relationship (QSAR) involving 26 seconucleosidenitrosourea compounds having anticancer activity against murine adenocarcinomas of the colon 15A (MAC 15) [1].

Shrivastava's objective of the research article is to perform *in-silico* structural assessment analysis of protein database entries of Plasmodium falciparum lactate dehydrogenase (PFLDH) enzyme, an important target for designing anti-malarial drugs. This study used ANOLEA energy assessment and Swiss model to analyze Ramachandran plot. Results of the study concludes that out of all the PDB entries used, PBD 1T24 was found to be the best suit for carrying out structure based drug design (SBDD) studies [2].

Author Rath, in his article proposed the use of QSAR analysis to determine the antimicrobial effects of novel and untested QACs and QAC-like, structures for further testing. The study identified several promising antimicrobial compounds. Further, the study suggests diversifying the availability of QACs to develop better disinfectants, create more environment friendly compounds, and help to stall, or even halt, the development of antimicrobial resistance [3].

References

1 Noorbatcha IA, Samsudin N, Salleh HM (2016) Quantum Chemical Structure Activity Studies of Anticancer Activity of Seconucleoside Nitrosourea Analogs. Chem Inform 2: 1.

2 Shrivastava A, Kumar J, Akhter M (2016) *In-Silico* Assessment of Various PDB Entries of PFLDH Enzyme for their Use in SBDD. Chem Inform 2: 1.

3 Rath EC, Bai Y (2016) Quantitative Structure-Activity Relation Study of Quaternary Ammonium Compounds in Pathogen Control: Computational Methods for the Discovery of Food Antimicrobials. Chem Inform 2: 1.