Trends in Phytochemical Research (TPR)

Journal Homepage: http://tpr.iau-shahrood.ac.ir

Guest Editorial

Computer-aided phytochemical research

Satyajit D. Sarker ✉ and Lutfun Nahar

Medicinal Chemistry and Natural Products Research Group, School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, James Parsons Building, Byrom Street, Liverpool L3 3AF, UK

© 2017 Islamic Azad University, Shahrood Branch Press, All rights reserved.

Nowadays computation or computational aspects are present almost in everything we do. Over the last couple of decades, the advancement in computer science and their applications in our everyday life has simply been phenomenal, and has impacted positively on how we carry out research. Chemistry has already embraced computation and various mathematical modelling to solve various research questions and to develop new methods, which have finally led to the establishment of a recognised branch in Chemistry, known as Computational Chemistry.

We now define computation chemistry as a branch of chemistry that uses computer simulation to assist in solving chemical problems. It utilises various methods of theoretical chemistry, embedded into efficient computer programmes, mainly to calculate the structures and properties of molecules and solids, e.g., electronic structure determination, geometry optimizations, frequency calculations, transition structures, docking, electron and charge distribution, rate constants and many more. Some common softwares used in computational chemistry are Gaussian 94, GAMESS, MOPAC, Spartum and Sybyl.

In recent years, we have observed a noticeable increase in the incorporation of computational techniques, artificial intelligence and mathematical modelling in phytochemical research, especially in screening plant materials, plant metabolomics, chemical fingerprinting, chemical taxonomy, phylogenetic studies, prediction of pharmacological and toxicological properties (virtual screening or *in silico* studies), and automated structure determination of phytochemicals based on spectroscopic data. There are several articles published on the use of computational approaches to solve a number of issues in phytochemical research (Nuzillard and Massiot 1991; Stortz and Cerezo 1992; Rollinger et al., 2005; Jeeshna and Paulsamy 2011; Barlow et al., 2012; Desai and Gore 2012; Ningthoujam et al., 2014; Das et al., 2017), and relevant useful methodologies and techniques have been outlined therein.

In most cases, the introduction of computer-aided approaches is saving time and money associated with phytochemical research, ranging from bioactive compound discovery to identifying the metabolomes. Whilst it is envisaged that the impact of computational methods in phytochemical research will grow steadily over the coming years, and will probably totally transform the way we carry out phytochemical research today, computer-aided phytochemical studies can certainly be considered as one of the major current trends in phytochemical research.

References

Barlow, D.J., Buriani, A., Ehrman, T., Bosisio, E., Eberini, I., Hylands, P.J., 2012. *In silico* studies in Chinese herbal medicines' research: evaluation of *in silico* methodologies and phytochemical data sources, and a review of research to date. J. Ethnopharm. 140(3), 526-534.

Das, S., Laskar, M.A., Sarker, S.D., Choudhury, M.D., Choudhury, P.R., Mitra, A., Jamil, S., Lathiff, S.M.A., Abdullah, S.A., Basar, N., Nahar, L., Talukdar, A.D., 2017. Prediction of anti-Alzheimer's activity of flavonoids targeting acetylcholinesterase *in silico*. Phytochem. Anal. In press.

Desai, N.S., Gore, M., 2012. Computer aided drug designing using phytochemicals-bacoside A3 and myricetin and nitric oxide donors-*S*-nitroso-*N*-acetylpenicillamine and nitroglycerin as a potential treatment of pancreatic cancer. J. Comput. Sci. Sys. Biol. 5(1), 1-8.

Jeeshna, M.V., Paulsamy, S., 2011. Phytochemistry and

✉ Corresponding author: Satyajit D. Sarker
Tel: 0151-231-2096, Fax: 0151-231-2170
E-mail address: S.Sarker@ljmu.ac.uk

bioinformatics approach for the evaluation of medicinal properties of the herb, *Exacum bicolor* Roxb. Inter. Res. J. Pharm. 2(8), 163-168.

Ningthoujam, S.S., Choudhury, M.D., Potsangbam, K.S., Chetia, P., Nahar, L., Sarker, S.D., Basar, N., Talukdar, A.D., 2014. NoSQL data model for semi-authomatic integration of ethnomedicinal plant data from multiple sources. Phytochem. Anal. 25(6), 495-507.

Nuzillard, J.M., Massiot, G., 1991. Computer-aided spectral assignment in nuclear magnetic resonance spectroscopy. Anal. Chim. Acta. 242(1), 37-41.

Rollinger, J.M., Bodensieck, A., Seger, C., Ellmerer, E.P., Bauer, R., Langer, T., Stuppner, H., 2005. Discovering COX-inhibiting constituents of *Morus* root bark: activity-guided versus computer-aided methods. Planta Med. 71(5), 399-405.

Stortz, C.A., Cerezo, A.S., 1992. The ^{13}C NMR spectroscopy of carrageenans: calculation of chemical shifts and computer-aided structural determination. Carbohyd. Poly. 18(4), 237-242.