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Guest Editorial

Computer-aided phytochemical research

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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, Spartan 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.

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