Editorial

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Innovative Research Works on Chemical Informatics

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EDITORIAL NOTE

Cheminformatics (also known as chemoinformatics) refers to use of physical chemistry theory with computer and information science techniques — so called "in silico" techniques — in application to a range of descriptive and prescriptive problems in the field of chemistry, including in its applications to biology and related molecular fields[1]. Such in silico techniques are used, for example, by pharmaceutical companies and in academic settings to aid and inform the process of drug discovery, for instance in the design of well-defined combinatorial libraries of synthetic compounds, or to assist in structure-based drug design. The methods can also be used in chemical and allied industries, and such fields as environmental science and pharmacology, where chemical processes are involved or studied[2].

Cheminformatics has been an active field in various guises since the 1970s and earlier, with activity in academic departments and commercial pharmaceutical research and development departments. The term chemoinformatics was defined in its application to drug discover, for instance, by F.K. Brown in 1998:

Chemoinformatics is the mixing of those information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of drug lead identification and optimization[3].

Since then, both terms, cheminformatics and chemoinformatics, have been used,although, lexicographically, cheminformatics appears to be more frequently used,despite academics in Europe declaring for the variant chemoinformatics in 2006. In 2009, a prominent Springer journal in the field, the Journal of Cheminformatics, was founded by transatlantic executive editors, giving yet further impetus to the shorter variant[4,5].

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