MS045.O02

Crystallography as an introduction to cheminformatics

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Information management and its subsequent analysis to derive new knowledge is ubiquitous in the digital age, with companies such as Google and Amazon being built on such foundations and becoming hugely successful as a result. As a research discipline chemistry is rather behind in this area – there is not a significant culture of the whole discipline working coherently to generate large bodies data that can be used to perform further scientific research. In part this can be attributed to a lack of understanding and education as to how and why Cheminformatics might be used. Moreover, Cheminformatics is used at a significant level in chemical industries and employers are anxious to recruit graduates with a good understanding of the principles – irrespective of whether it is put into practice or not, as it is important for everyone in the organisation to understand why collecting and using data is important.

Fundamentally Cheminformatics is the application of computing to chemical data to transform it into information and ultimately knowledge. The crystallographic community has in fact been doing this for many years and can clearly act as an example to others. The community has been collecting crystal structures for over 50 years and in that time has gone on develop tools that can make more of that data and which have their own independent research value.

The Chemistry department at Southampton has been involved in Cheminformatics research for a number of years and in order to address the lack of skills and understanding in this area has developed a module to teach it to undergraduate and masters level students. Crystallography is used as a familiar example to introduce students to the end-to-end concepts – from collating individual data (structures) through to the application of knowledge bases to drug design. This talk will describe the module as a whole and illustrate the way in which an understanding of chemical structure, data management and informatics in crystallography is used to teach the fundamental concepts of Cheminformatics.

Keywords: Cheminformatics, database, education