

The Impact of e-Science

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Chemistry is an "information science" and at its heart is the relationship between structure and properties. To handle the rapid explosion in the number of structures made available by combinatorial chemistry knowledge management techniques based on a computational infrastructure are required. The "CombeChem" e-Science project considers aspects of the combinatorial chemistry approach from the design of drugs through to selection solid-state materials for delivery. e-Science concepts will be illustrated by a discussion of single crystal structure determination in the context of polymorph screening, computational grids for drug protein binding studies, the importance of good statistical design of the experiments and the acquisition of metadata in a laboratory to ensure this data carries adequate provenance. I will attempt to show how a Grid can provide the necessary computing infrastructure to ensure that the quantities of information can be handled automatically and smoothly to provide the basis for collaboration between disparate users.