

Chemical databasing technologies and databases, have been available for many years. At this point it would be expected that trends stabilize. While there are dominant commercial chemical databases such as CAS and Reaxys, in terms of technologies and publicly accessible databases there has been a continuous increase in the variety of database engines and chemistry content offerings via databases. This presentation will review the history of chemical databases and will cover present trends. We will analyse the challenges in general databasing technologies which are attributed to the current trends in Big Data and Semantic Web and will show how those challenges and trends affect technical solutions applied to chemistry.

The Royal Society of Chemistry has participated in a number of national and international grants allocated to the construction of large scale chemical information management systems including examples such as the Innovative Medicines Initiative project know as Open PHACTS, the PharmaSea project to identify novel antibiotics from the ocean and the National Chemical Database Service, a hub of cheminformatics services and related content made available to chemists in UK academia. We will talk about the specifics of each project and present the technical and scientific solutions that have helped make these successful.

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