

- T.C. Terwilliger, *IUCrJ*, 4:87-99 (2017).
6. A.L. Spek, *Acta Crystallogr. Sect. D Biol. Crystallogr.*, 65:148-155 (2009).
 7. International DOI Foundation, DOI Handbook <http://www.doi.org/hb.html> (Accessed Jan 20, 2017).
 8. ORCID | Connecting Research and Researchers <https://orcid.org/> (Accessed Jan 20, 2017).
 9. C. Groom, New Communications with the New CSD <http://www.ccdc.cam.ac.uk/Community/blog/2016-03-15-new-communications-with-the-new-csd/> (Accessed Jun 20, 2016).
 10. I.J. Bruno, G.P. Shields, R. Taylor, *Acta Crystallogr. Sect. B Struct. Sci.*, 67:333-349 (2011).
 11. C.R. Groom, T.S.G. Olsson, J.W. Liebeschuetz, D.A. Bardwell, I.J. Bruno, F.H. Allen, 5 Mining the Cambridge Structural Database for Bioisosteres, in: N. Brown (Ed.), *Bioisosteres in Medicinal Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2012: pp. 75-101.
 12. P.T.A. Galek, E. Pidcock, P.A. Wood, N. Feeder, F.H. Allen, Navigating the Solid Form Landscape with Structural Informatics, in: *Comput. Pharm. Solid State Chem.*, John Wiley & Sons, Inc, Hoboken, NJ, 2016: pp. 15-35.
 13. S. Heller, A. McNaught, S. Stein, D. Tchekhovskoi, I. Pletnev, *J. Cheminform.*, 5:7 (2013).
 14. H.E. Pence, A. Williams, *J. Chem. Educ.*, 87:1123-1124 (2010).
 15. E. Bolton, Y. Wang, P. Thiessen, S. Bryant, PubChem: Integrated Platform of Small Molecules and Biological Activities, in: R.A. Wheeler, D.C. Spellmeyer (Eds.), *Annual Reports in Computational Chemistry*, Volume 4, Elsevier, Oxford, UK, 2008: pp. 217-240.
 16. wwPDB, Data correspondences between the PDB and CSD archives now available. <http://wwpdb.org/news/news?year=2015#29-July-2015>.

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Big Data in Chemical Industry

by Dr. B. Saha

Big data with advanced analytical software is now being used by many chemical companies to improve business performance.

There are several areas where “Big Data” has started playing an important role in chemical industry. This includes Manufacturing, Supply Chain Management, Marketing, Innovation, and Human Resource Management.

In manufacturing, use of Big Data is helping companies to improve productivity and efficiency. In Supply Chain Management, cost optimization is being done through data analysis of freight, raw material prices, procurement schedules, and storage costs, etc. Big data with advanced analytical software is providing Marketing departments insight into product trends, demand, future customer requirements, and so on. Another important area in which Big Data usage is changing industry is in pricing. Pricing decisions depends on a multitude of variable factors, such as the cost of raw materials, exchange rates, utility costs, competitors’

prices, market demand, etc. Big Data Analytics has started playing an important role in these decisions, as well as in demand forecasting, which can have a major impact on the success of businesses.

Big data is helping innovation management by allowing the analysis of the vast data available on chemicals and their properties, including biological activities. In Human Resource Management, the analysis of data helps to identify parameters impacting job satisfaction, employee retention, and many other issues.

There are more than 15 software companies in India who have specialized in Big Data Analytics. In the Indian chemical industry, it is now felt that one must invest in Big Data and Analytics, which will bring immense benefit to the organization.

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