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Data and compute intensive escience approaches in computational medicinal chemistry

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eScience is an inherently multi-disciplinary pursuit concerned with the use of compute-intensive methods to enable data-driven science. The challenge of eScience is to ensure that the most value can be gained from all new scientific endeavors by using information technology (IT) to improve experimental design, data management, data analysis and communication as well as to model and simulate complex systems and behaviors. Medicinal chemistry, like most scientific disciplines, is becoming increasingly data-intensive and dependent on our capacity to manage and exploit growing data resources. In particular, there is increasing need for drug-discovery organizations to enable decision making that is informed by the growth of their internally generated data and its integration with external data. This talk will explore the latest developments in eScience in the context of drug-discovery and how advanced computing and data-driven methods will increasingly impact chemical exploration and rational design.

Biography

Scott James Lusher worked in pharmaceutical R&D (Organon, Schering-Plough and Merck) for ten years (2001-2011) providing the molecular basis and rationale for the selection and design of NCEs within cross-disciplinary projects. Additionally, he had a role ensuring the strategic management and project implementation of molecular informatics within research. He joined the Netherlands eScience Center in 2011 as part of its management team and is currently Director Applied eScience developing new scientific applications of ICT. He has a part-time appointment at the Radboud University Medical Center and has a PhD in computational drug design from the same institute.