High-throughput, Grid Based Prediction of ADMETox Parameters Leveraging the Unused Computational Capacity of Enterprise IT Infrastructure

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Pharmaceutical companies are facing the challenges that modern drug discovery requires precise "high-throughput" *in silico* systems that are able to predict the ADMETox properties for millions of structures in a very short time. On the other hand, mergers in the pharmaceutical industry demand the secure integration of geographically distributed information and computation resources. These challenges make indispensable the usage of GRID systems in enterprise infrastructures. As a consequence, chemical applications developed for traditional environments have to be redesigned to meet the requirements of this new technology.

ADMEToxGrid is an enterprise Grid system designed to predict molecular properties for extremely large number of compounds in a reasonable time and in a secure manner. To achieve the requested high throughput, the system can utilize computational clusters, as well as exploit the unused capacity of the desktop computers located at the different sites of the enterprise. The advanced tracking of prediction tasks and packages ensures the safe and reliable operation of the system, and the predicted properties can automatically be integrated into the proprietary database of the company.

The poster describes the ADMEToxGrid system, detailing the features provided by the technologies implemented in the grid framework. In addition, we present the first experiences with the application of the system, showing the results of benchmark tests.