Development of an extensible system for the capture and storage of experimental enzyme kinetics data

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Abstract
A number of resources are available to the community providing access to enzyme kinetic parameters. Many of these sources have been compiled through extensive manual data mining of published papers. However, there are few resources covering the storage of the original, raw experimental data sets from which these parameters were calculated.

We introduce here a relational database for the storage of experimental enzyme kinetics data. The implementation of an extensible Java data model is also discussed, from which an automated wizard has been generated allowing data submission directly from the BMG Labtechnologies NOVOstar instrument software. This submission tool exploits the soon-to-be-released libSBML[1] v3.0, which greatly facilitates the data modeling of enzyme kinetics experimental metadata. Existing web services are also exploited, allowing the user to annotate experimental enzyme kinetics data with standard ontological terms that ultimately facilitate the generation of MIRIAM[2] compliant models.

This combination of relational database repository, data model and submission tool can be extended further to integrate with any number of manufacturer instruments covering a range of spectrometric techniques.

Furthermore, it is shown that existing databases containing enzyme kinetics data can be integrated with the experimental data repository, providing users of kinetic parameter databases with the ability to view the experimental data on which they are based, giving increased user confidence in the parameters and/or allowing users to calculate

their own parameters or to fit them to different kinds of kinetic mechanism.

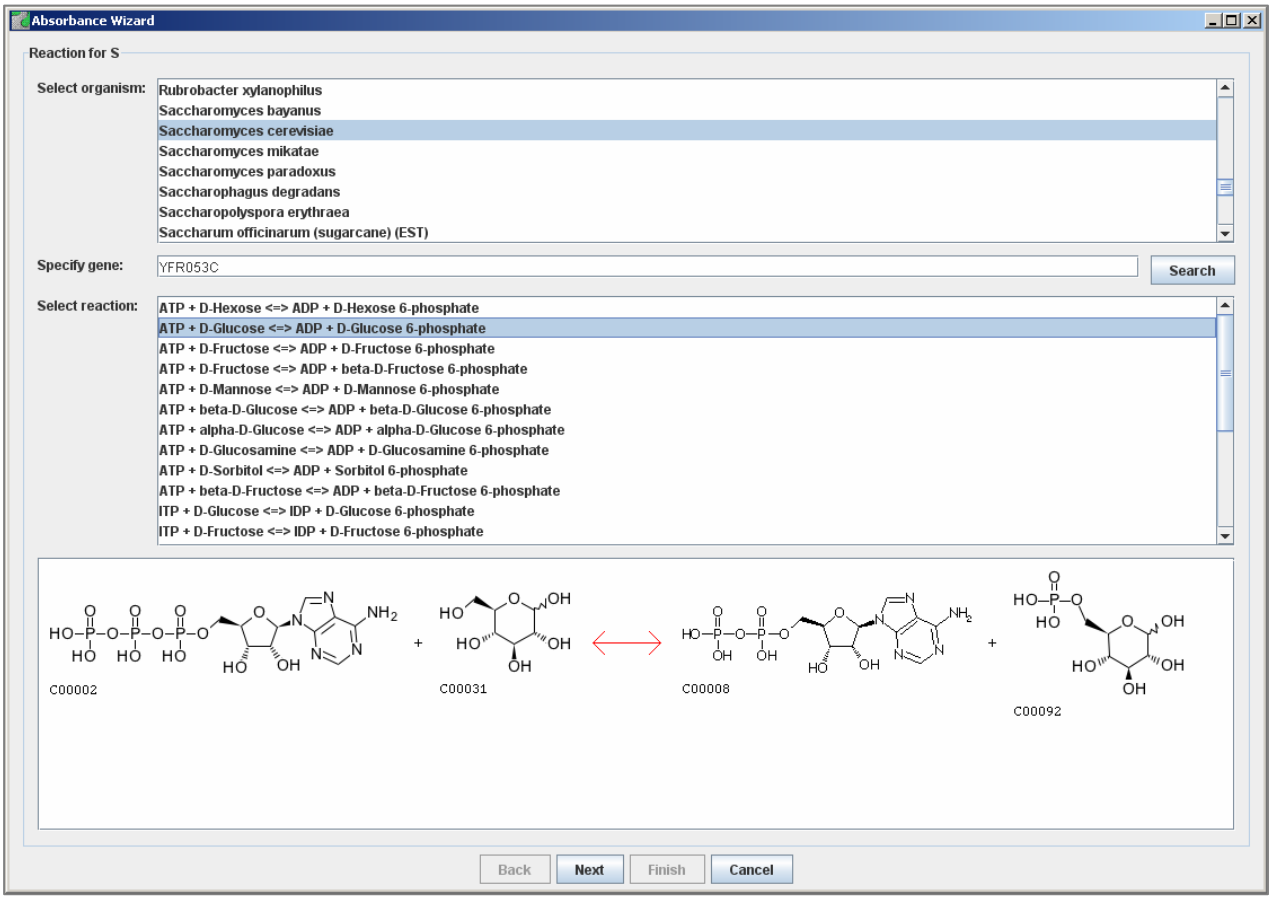

Figure 1: The Absorbance Wizard submission tool allows specification of species, gene and reaction, utilising the existing web services of GO[3], ChEBI[4] and SBO[5] to ensure the use of consistent ontological terms.

References

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