

Poster presentation

## Automating QSAR expertise

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The Discovery Bus, a multi-agent software system designed for automating aspects of Molecular Design, particularly expert decision making, is described. It extends approaches aimed at automating the processing of drug discovery information but where control remains with the human expert, to automating the "tacit knowledge" of the expert and best practice, which we model as a workflow, and experience, which we model as alternative, competing processing nodes in the workflow.

An example application of this architecture to automating QSAR best practice will be described with examples of specific models as well as performance metrics for large numbers of QSAR datasets, multiple descriptors and alternative learning methods will be described. Recent extensions of the approach to multi-objective, reverse QSAR will also be covered. These extensions use a particle swarm algorithm to identify Pareto Solutions for multiple QSAR models in descriptor space, following by an evolutionary approach to generate novel structures proximate those solutions.

### References

1. The discovery bus. . [<http://www.discoverybus.com>]