Celltech Integrates Spotfire and Daylight for Superior Chemistry Analytical Platform - A Case Study

Summary

Celltech chose DayCart as the Oracle chemistry cartridge on which they would build their powerful registration based on DayCart's superior performance, sophisticated cheminformatics, and open architecture that allows scientific software from other vendors to tie in easily. DayCart's implementation enables a single copy of the corporate chemical data to be accessed from the desktop of all NCE discovery scientists within Celltech.

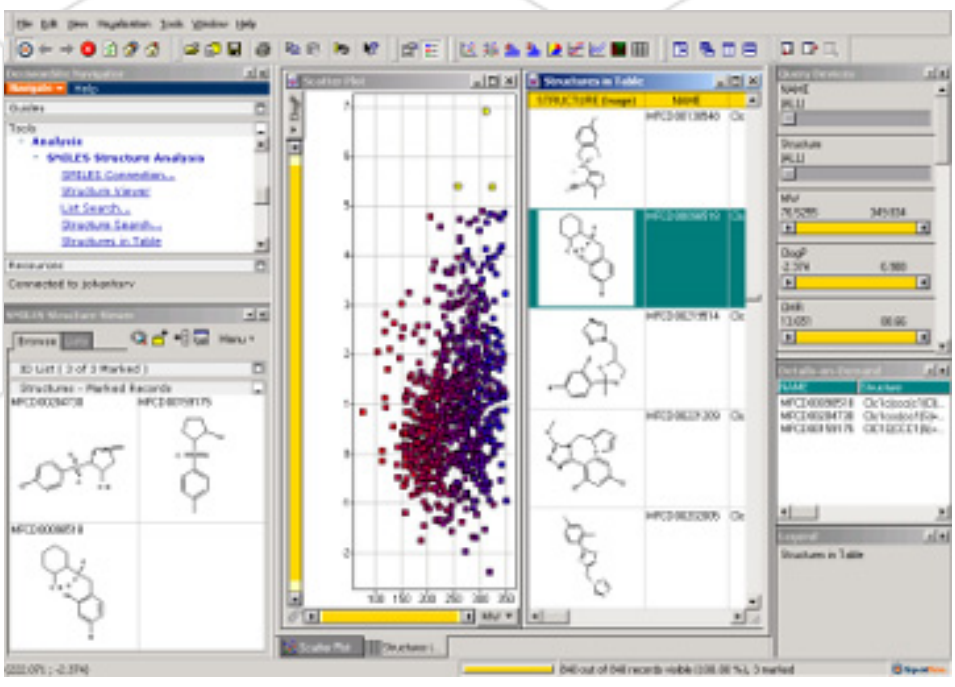

Fig. 1. Spotfire DecisionSite compound discovery application using Daylight DayCart.*

As part of the plan, Celltech has integrated Spotfire tightly into this system, enabling scientists to search and visualize chemical structures stored in DayCart in conjunction with data analysis in Spotfire DecisionSite. The open standards-based chemistry platform provides five distinct tools built by Spotfire's Professional Services team:

SMILES Connection Tool

SMILES is a language initially designed by Daylight and now an international standard for structure representation. It is the language used to store structures in DayCart. The SMILES Connection Tool is a dialog that allows the user to specify the chemistry source: either connect to a DayCart database or display structures from a SMILES column in the Spotfire dataset.

Structure Viewer Tool

The Structure Viewer Tool is used to view structures, either single compounds or compounds from lists. The compounds viewed could be the compounds corresponding to the currently selected records in the Spotfire visualization or a hit list from a database search (e.g., structure- or list-based search).

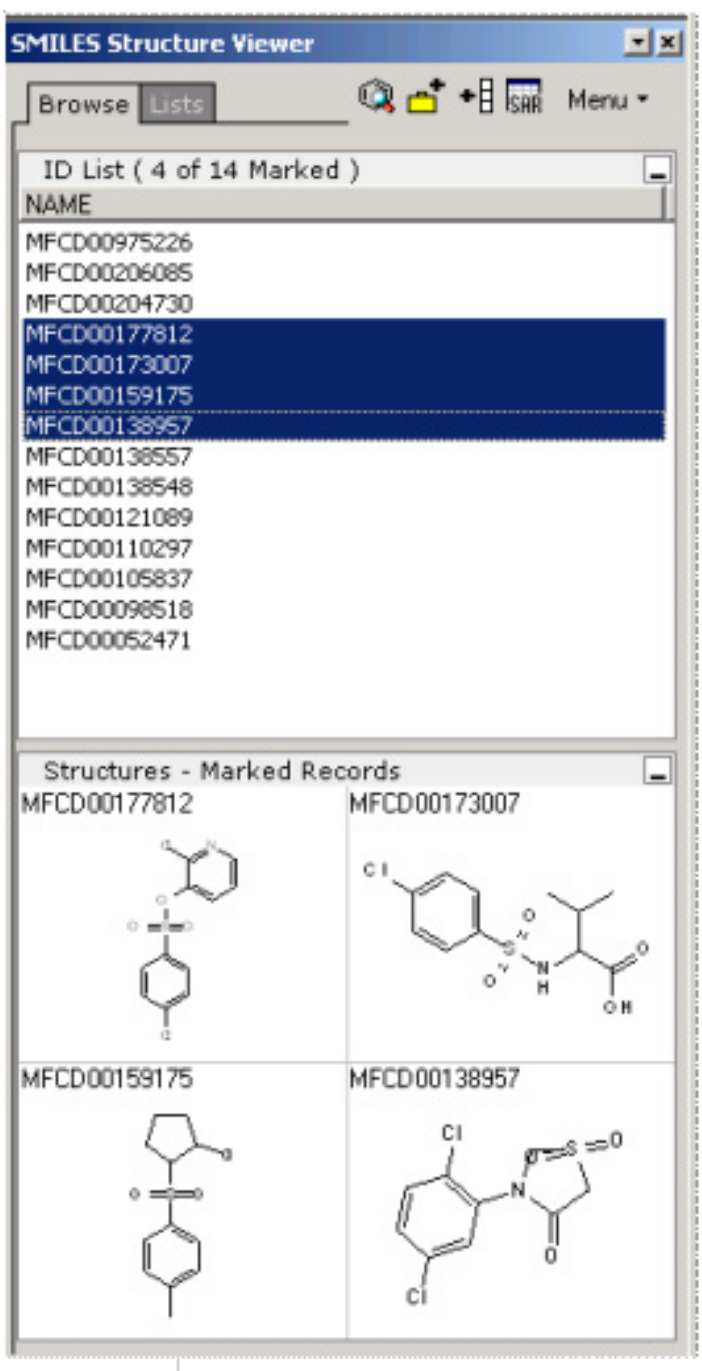

Fig. 2. The SMILES structure viewer in Spotfire DecisionSite.*

Structure-Based DayCart Search Tool

The Structure-Based DayCart Search Tool (or structure search tool) is a dialog where the user is able to perform substructure and exact match structure searches on a DayCart database. The search is performed against the database that the user has specified through the Connection Tool. In the dialog, the user has the possibility

to specify which type of search to perform, and with which structure to perform the search.

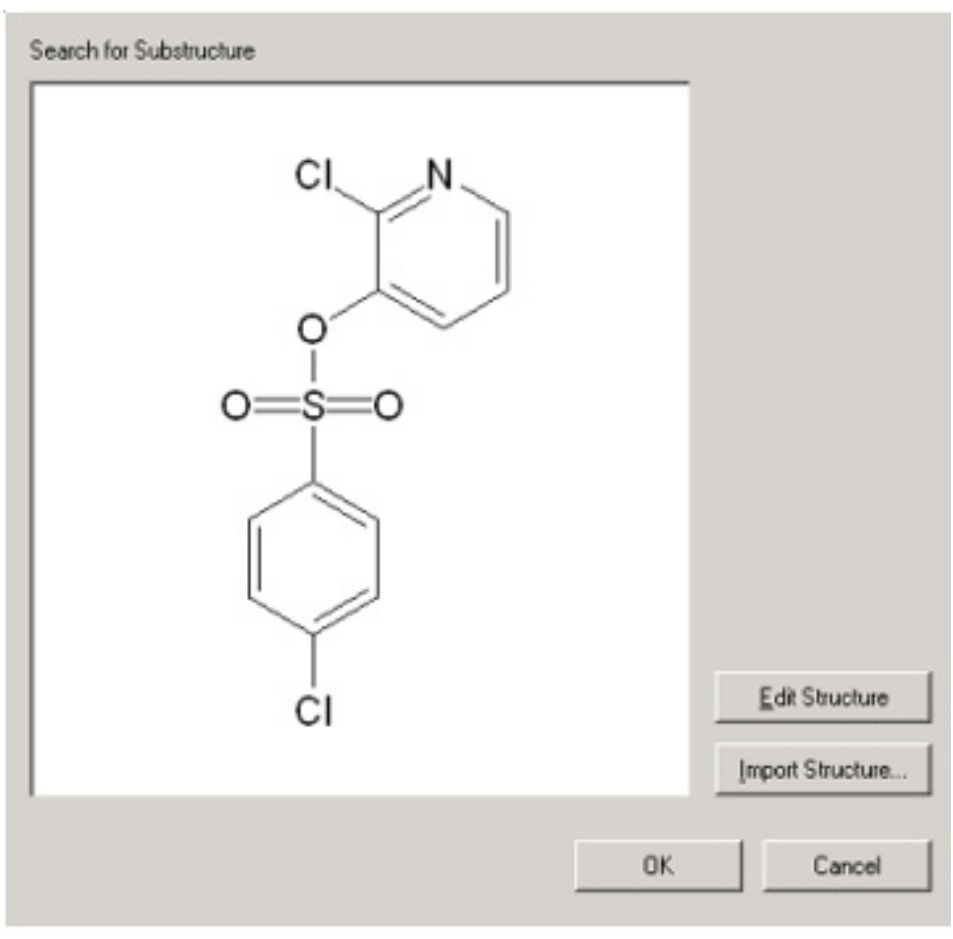

Fig. 3. Substructure search in DayCart using Spotfire DecisionSite.*

Structure-Based DayCart Search Tool List-Based DayCart Search Tool

The List-Based DayCart Search Tool is a dialog where the user can perform searches on a DayCart database based on a list of compound identifiers or a selection in the Spotfire dataset. The tool also allows retrieval of all structures in the database.

Structures in Table Tool

The Structures in Table Tool allows the user to quickly and simply add a compound structure column to a table visualization in Spotfire. If a table visualization exists in the Spotfire session when the tool is launched, the structure column is added to that visualization, otherwise a new table is created.

With these five tools, Celltech has bridged their intuitive visualization and analytical environment to the high performance and chemical intelligence of Daylight's enterprise cheminformatics system. This combination underpins Celltech's state-of-the-art research capabilities, and also serves as the foundation of a Daylight-Spotfire complementary technology partnership with many more possibilities.

David M. Parry, Section Leader - Exploratory Chemistry at Celltech, is enthusiastic about the Daylight-Spotfire integration and forward collaboration. "The marriage of the powerful data visualisation and analysis capabilities of Spotfire alongside Daylight's DayCart chemical cartridge for Oracle allowed Celltech to build a no-compromise data retrieval, visualisation, and analysis solution for NCE discovery," said Parry. "Celltech continues to be very excited by the numerous opportunities provided by this powerful and flexible combination for internal cheminformatics initiatives."

In the months ahead, Daylight and Spotfire will be working with customers to design more tools and applications based on this open chemistry platform, delivering the benefit of their collaboration directly to the scientists who have demanded it.