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Integration of ACD/Labs calculators and Symyx® Draw promotes improved efficiency, productivity in research and discovery

No-charge add-ins integrate Symyx Draw with ACD/Labs' nomenclature software, physical property calculators and NMR predictors

SANTA CLARA, CA and TORONTO, ON (October 8, 2007)—Researchers using Symyx Draw (previously MDL Draw) now have the option to increase the power and potential of the popular chemical drawing software by adding no-charge add-ins that calculate physical properties, generate IUPAC nomenclature and predict NMR chemical shifts. Add-ins available from Symyx and Advanced Chemistry Development, Inc. (ACD/Labs) enable researchers to generate and store this relevant data within the Symyx® ISENTRIS® environment.

The Symyx Draw calculator add-ins enable researchers to calculate molecular properties such as pKa, logD, logP and solubility, generate IUPAC names and predict ¹³C NMR and ¹H NMR chemical shifts and coupling constants, as well as 2D NMR spectra without leaving the ISENTRIS environment, resulting in smoother workflows and increased productivity. Bioconcentration factor, adsorption coefficient and boiling point calculators round out the suite of available tools.

ACD/Labs Name, PhysChem and NMR predictors are recognized as industry-standard tools. The outstanding accuracy of the prediction algorithms has been refined over more than 12 years of continuous development by ACD/Labs.

"It has made a lot of sense to combine our strengths," said Val Kulkov, CEO of ACD/Labs. "Through the ISENTRIS Alliance, we are partnering with Symyx to provide integrated solutions that offer researchers chemical naming and spectral and physicochemical property predictions out-of-the-box with ISENTRIS."

"Symyx's partnership with ACD/Labs through the ISENTRIS Alliance has resulted in a high-value win for our mutual customers," said Tim Campbell, President of Symyx Software. "Integrating ACD/Labs applications into Symyx Draw promotes a powerful set of tools from a valued partner while improving the day-to-day efficiency and productivity of researchers. This important development illustrates how ISENTRIS partners are bringing interesting and valuable functionality to researchers."

Go to www.acdlabs.com/mdldraw to request a no-charge download of the ACD/Labs add-ins.

See how easy it is to extend Symyx Draw with functionality that meets your needs. Sign up for an informative Web Seminar entitled "ACD/Labs and Symyx Draw: Adding scientific calculators to premier drawing tool," which will be jointly hosted by Symyx and ACD/Labs on October 30, 2007. Visit www.mdl.com/webinars for additional details and times.



In addition to the above ACD/Labs add-ins, other calculators available at no charge from within Symyx Draw include: simple structure-to-InChI, InChI-to-structure and SMILES-to-structure conversion tools; a 'Calculate-as-you-draw' add-in that calculates structural properties on-the-fly using Symyx® Cheshire® scripts; a Bioavailability add-in that uses Cheshire to calculate properties and plot them using a third-party .NET graphing control; an Isotopomer Distribution add-in that predicts molecular ion peaks using Cheshire and the same high-performance graphing control; and a Send-to-DiscoveryGate add-in that enables researchers to conduct DiscoveryGate® searches from within Symyx Draw. Go to www.mdl.com/support/developer/mdl-draw to download any of the additional Symyx Draw add-ins and sample code at no charge.

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