

Advanced
Chemistry
Development

ACD/Labs

What's New with ACD/PhysChem Suite Version 12.0

For more than a decade, ACD/Labs has been fully dedicated to building integrated solutions that enable data transfer and connection within chemical organizations. We remain committed to the adoption and creation of the latest technological and industrial advances, empowering our customers' research and development efforts with the foremost chemical capabilities. Each year, we release newer versions of our software to provide enhanced capabilities and superior integration between existing and new technologies.

New capabilities for ACD/PhysChem Suite 12.0 have resulted from collaboration with our users, as well as feedback from industry experts. We appreciate your input and encourage you to contact us with ideas or suggestions for new features by visiting support.acdlabs.com. In addition, we invite you to join us at one of the seminars we will be holding throughout the year to discuss our products and learn more about the current version. Visit www.acdlabs.com/events/ for a list of upcoming events.

Among the key features for ACD/PhysChem Suite presented below, are:

ACD/PhysChem Suite (*amalgamation of all predictor products*)

- All-in-one Log P , Log D , Solubility, p K_a , and Boiling Point combined predictor product
- Enhanced p K_a display of ionized species
- Improved p K_a prediction model

General improvements to all PhysChem products

- Improved user training tools for all ACD/Labs PhysChem databases
- Updated QuickReport tool



ACD/PhysChem Suite

All-in-one logP, logD, solubility, pK_a, and boiling point combined predictor product

The individual PhysChem predictor modules for logP, logD, solubility, pK_a, and boiling point have been combined into a single product: ACD/PhysChem Suite. This includes the full capabilities of the individual predictor modules.

pK_a Algorithm (For all relevant products generating or using pK_a property)

Enhanced pK_a display of ionized species

The pK_a model predictions now provide relative abundance data for the ionized species for a specific pH. The relative abundances of the ionic species was previously only available as part of our solubility prediction model details.

The ability to predict the relative abundances of ionic species at different pHs enables users to determine which structure form should be used for computational predictions. Knowing the right ionized species is also valuable for assessing the results from QSAR models and high-throughput screening (HTS) hits.

- Table of Relative Abundances for ionic species
 - User definable pH scale
 - User definable ionic species

Improved pK_a prediction model

The ACD/Labs pK_a prediction model was updated to provide better accuracy and to expand the applicable chemical space covered.

Several of the pK_a-models' Hammett equations were further refined along with the addition of new reaction centers. The data utilized for enhancing the pK_a models were obtained from research collaborations with pharmaceutical companies that generate lead compounds.

Training (All ACD/Labs PhysChem databases)

Improved User Training tools

The ability to incorporate your internal proprietary data to improve model predictions is a critical aspect of ensuring that the best possible physicochemical predictions are provided. The System Training and Accuracy Extender tools have been refined in version 12 to improve their performance.

ACD/Labs User Training tools are provided with our PhysChem software so that users can expand and improve our PhysChem prediction models with proprietary data. The performance of these tools has been enhanced to reduce the time required to build the training set, along with reducing the calculation time of our models when utilizing this user training.

- Improved speed for importing User Data
- Reduced calculation times per molecule when User Training is utilized



Reporting (All ACD/Labs desktop PhysChem predictors)

Updated QuickReport tool

The QuickReport tool provides an interactive user-definable interface. The tool has been enhanced so that it now has two calculation modes: automatic and manual calculation.

The original version of QuickReport required that users switch between the ChemSketch window and the QuickReport tool in order to calculate the predicted properties. The user can now use the automatic calculation mode to see how the properties change as the structure is being drawn.

- QuickReport automatic calculation
- User definable time delay for calculation
 - User specified time delay
 - User definable prediction display

Additional Improvements

New customizable interface appearance & style

The interface style and appearance has been refreshed. The background color, buttons, and other graphic controls can be made to conform to the Windows setting, the classic ACD/Labs view, or you can create your own theme and preference.

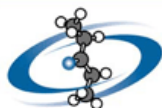
Launch different ACD/Labs applications from the Windows taskbar

Previously all ACD/Labs applications shared the same button on the Windows taskbar. Now, it is possible to expand the ACD/Labs button on the taskbar into separate buttons for each application.



To learn more about this product, please download our catalog from <http://www.acdlabs.com/download/catalogs/physchem.pdf> or visit our Web site (<http://www.acdlabs.com/physchemsuite/>).

Because ACD/Labs software is highly integrated, new features in connected modules may also be relevant. In particular, you may want to review information about ACD/ChemSketch ACD/Structure Design Suite, ACD/Structure Designer, and ACD/ChemFolder.



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