

**A d v a n c e d  
C h e m i s t r y  
D e v e l o p m e n t**

**ACD/Labs**

## What's New with ACD/Name 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/Name 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](http://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/](http://www.acdlabs.com/events/) for a list of upcoming events.

Among the key features of ACD/Name presented below, are:

- Set standard InChI options (updated IUPAC recommendation)
- Multiplication of different substituents—IUPAC bug fix
- Phasing out AZOXY naming conventions—Index Name
- Expanded conversion of non-systematic names to structures
- Name-to-Structure algorithm improvements
- Support InChI for V3000 SDfiles in ACD/Name Batch



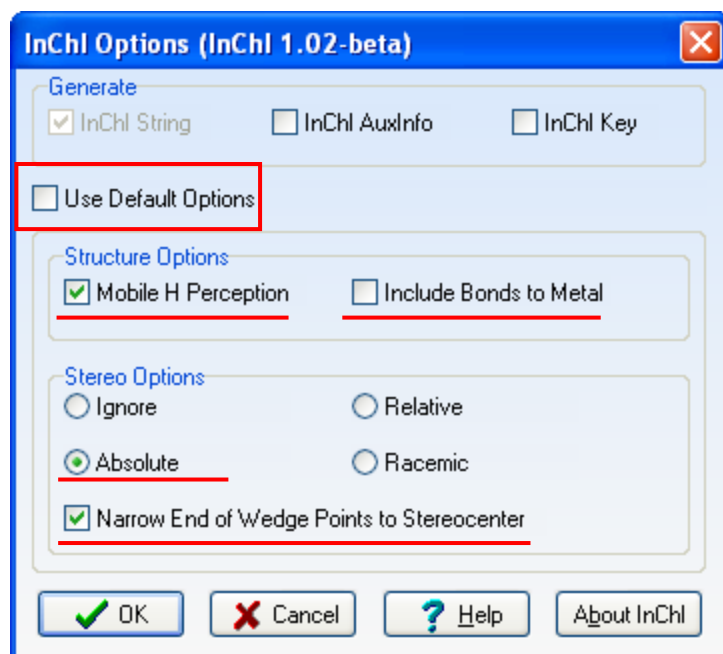
## IUPAC InChI Group Recommendations

Set standard *InChI options* (updated IUPAC recommendations)

New InChI options proposed by IUPAC were implemented. The options include:

- Mobile Hydrogen Perception (taking tautomerism into account)
- Excluded bonds to metal
- Absolute stereoconfiguration
- Taking into account the narrow ends of stereobonds only

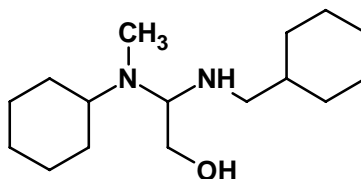
The IUPAC International Chemical Identifier (InChI™) is a non-proprietary identifier enabling unambiguous identification of chemical substances for electronic handling of chemical structural information. These new IUPAC options for InChI reflect the decisions made by the IUPAC InChI project group, and are intended to increase the role of InChI and InChI key as a universal structure identifier



## IUPAC Nomenclature

*Multiplication of different substituents*

Some substituents that differ only in enclosing marks were multiplied incorrectly as if they were the same. This bug was corrected.



Previously: **2,2-bis[cyclohexyl(methyl)amino]ethanol**

Now: **2-[(cyclohexylmethyl)amino]-2-(cyclohexyl(methyl)amino)ethanol**

**IUPAC rules in CHM format**

With Windows Vista, Microsoft discontinued support for the HLP files format that was being used to access IUPAC rules from ACD/Name. As a result, the rules could not be displayed in ACD/Name for computers using the Vista operating system.

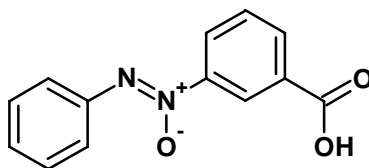
To remedy this situation, the rules were reformatted to CHM format. This new format is fully supported and offers better display, navigation, and search capabilities than the HLP files.

**CAS Index Name Nomenclature**

The majority of changes in naming principles introduced by Chemical Abstract Service (CAS) in November 2006 were implemented as part of the version 11 update. Version 12 continues to keep the naming algorithm up to date with current recommendations.

**New Index Rule: No More AZOXY**

Starting in 2007, CAS discontinued specific naming conventions for nitrogen containing groups in favor of more systematic names. One such group is AZOXY, which is now being phased out.



Previously: **benzoic acid, 3-(phenyl-*NNO*-azoxy)-**  
 Now: **benzoic acid, 3-(1-oxido-2-phenyldiazenyl)-**

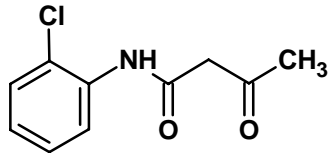
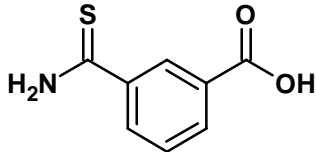
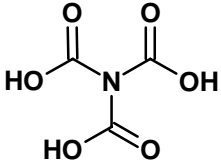
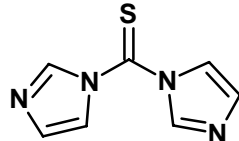
**Name to Structure Conversion****Expanded ACD/Dictionary improves conversion to non-systematic names**

With the addition of over 9000 trivial and systematic names and registry numbers for important chemical substances in ACD/Dictionary, and through expanded internal data files, the range of non-systematic names that can be converted to chemical structures is greatly expanded.

Name Input	Result in 11.0	Result in 12.0
Zaluzanin C	Cannot Recognize Name	
203-607-0 [EINECS number]	Cannot Recognize Name	

**Name-to-Structure algorithm improvement**

Improvement to the Name-to-Structure algorithms are ongoing and continue to expand the number of names that can be converted successfully.

<b>Behavior Name</b>	<b>Result in 11.0</b>	<b>Result in 12.0</b>
<i>Incorrect structure</i>		
2'-chloroacetoacetanilide	Wrong	
<i>Carbamothioyl recognition</i>		
3-carbamothioylbenzoic acid	No structure	
<i>Bad conversion of imidodicarbonic and nitrilotricarboxylic acid derivatives</i>		
nitrilotricarboxylic acid	No structure	
<i>Support prefixes for alternative names with thio (Se, Te) modifiers</i>		
1,1'-thiocarbonylbisimidazole	No structure	

**ACD/Name Batch** *(Purchasable separately from ACD/Name)***Generate InChI for V3000 SDfiles**

Version 12.0 of ACD/Name Batch supports V3000 molfiles and SDfiles for generation of names or alternate identifiers such as SMILES, InChI, and InChI keys.



## Additional Improvements

### ***Unnecessary warning for multiplicative nomenclature was removed***

An unnecessary warning that occurred for multiplicative nomenclature is no longer triggered inappropriately for name-to-structure.

### ***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 or the classic ACD/Labs view, or you can create your own theme and preference.

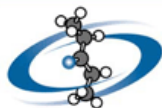
### ***Launch different ACD/Labs applications from the Windows taskbar***

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/namecat.pdf> or visit our Web site (<http://www.acdlabs.com/name/>).

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.



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