

ACD/Peptide Builder
Version 9.0 for Microsoft Windows

User's Guide

ChemBasic Goodie Description

Advanced Chemistry Development, Inc.

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Table of Contents

Before You Begin	ii
What are “Goodies”?.....	ii
Where Can I Get Them?	ii
About This Reference Manual	ii
<i>Advanced Understanding</i>	<i>ii</i>
For More Information.....	iii
<i>How to Contact Us</i>	<i>iii</i>
<i>Online Updates</i>	<i>iii</i>
1. Building 3D Peptide Structure.....	1
1.1 Amino Acid Shorthand Codes	1
1.2 Running ACD/Peptide Builder	2
1.2.1 <i>Amino Acid Code Representation</i>	2
1.2.2 <i>Input Text Code Source</i>	2
1.2.3 <i>Using an Existing Textbox with the Shorthand Codes</i>	3
1.2.4 <i>Entering Shorthand Code with a Form</i>	3
1.3 Example 1. SINGLE Letter Code Input with Textbox	4
1.4 Example 2: THREE Letter Code Input.....	7

Before You Begin

What are “Goodies”?

Goodies are additional tools that extend the functionality of ACD/ChemSketch. They are, actually, implemented as ACD/ChemBasic programs associated with the 22 supplementary ChemSketch buttons. ACD/ChemBasic is a special programming language that enables you to customize ACD/Labs software, and we think this is a great way to show off how useful it is—and at the same time make your ACD/ChemSketch even more versatile!

Note that you do not need to know anything about ACD/ChemBasic (although, if you wish, you can learn it by using the Goodies' code as example).

Where Can I Get Them?

To check if you already have Goodies, look for all .BAS files within your ACD/Labs example folder (\\EXAMPLES\CHEMBAS\GOODIES). If you don't find any, you can download them from our Web site free of charge at

http://www.acdlabs.com/products/chem_dsn_lab/goodies.html

They are easy to install and to use. Just follow the installation instructions provided at the aforementioned Web page and enjoy these new ACD/ChemSketch features. After installation, the Goodies tools are available as buttons on a toolbar you have specified.

About This User's Guide

This user's guide is provided in electronic form, readable with Adobe Acrobat software. If you cannot locate an index topic you need please do a text string search for the relevant word or phrase, or related words.

Advanced Understanding

This guide is intended to be a part of the technical documentation for ACD/Labs software. To study ACD/Labs products gradually, we recommend the following order of working through the technical documentation (all these documents are located in the ACD/Labs documentation folder \\DOCS\):

1. Documents for ACD/ChemSketch (CHEMSK_R.PDF and CHEMSK_T.PDF).
2. ACD/Dictionary (DICT.PDF) and ACD/3D Viewer (3D.PDF) to familiarize you with features of drawing and looking up the structures.
3. Peptide Builder User's Guide (current document).

For More Information...

To see the latest in ACD/Labs software and services, please visit our Web site at

<http://www.acdlabs.com/>

Our Web site is being accessed at the rate of tens of thousands of "hits" per day. There's a reason for this: much is offered through our Web site. As of Spring 2005, we offer free ChemSketch 8.0, a free ISIS 3D Add-in, free ChemDraw extensions, and a free 2-week demo key for "Interactive Laboratory" sessions where you can run test calculations using Java applets without purchasing software. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ACD/ChemSketch) available for download.

We are constantly updating the information on our Web site. The Web site will tell you at which scientific conferences you can visit the ACD/Labs booth. You can browse the Frequently Asked Questions page or drop in and "chat" on our newsgroup, which can also be reached via our web page.

If you would like to stay informed of the latest developments in chemical software at ACD/Labs, please be sure to sign up for e-mail broadcasts at our Web site page:

<http://www.acdlabs.com/feedback/mailing.html>

If you would like to participate in the ChemSketch newsgroup, please access:

<news://news.acdlabs.com/acd.public.chemsketch>

How to Contact Us

We are accessible through our Web site, phone, fax, and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability, and general issues should be directed to:

info@acdlabs.com

Technical and scientific support issues should be addressed by visiting:

<http://support.acdlabs.com>

Please tell us the name of the software purchaser; the product name, version number, build number, and license ID of the product you are contacting us about (from the **Help** menu, choose **About** to find this information); as well as a description of the problem you are having. If applicable, please tell us the name of the distributor from whom you purchased the software.

Online Updates

All the PC-based ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. The updates are small fixes, for example, bringing the actual version number of a program from 9.00 to 9.01. For more information on this, please refer to the document located in the ACD/Labs documentation folder, \\DOCSUP_CLNT.PDF, or contact our technical support department.

1. Building 3D Peptide Structure

The program accepts a peptide (protein) short-hand formula from either an input form or from a single textbox in the active ChemSketch page. Both 1-letter and 3-letter notations are allowed, but they cannot be mixed. The program will automatically check the input notation for any errors. By default, a right hand alpha-helix is assumed as the secondary structure for the whole peptide. However, the 3-letter notation can be extended to allow the user to indicate particular residues secondary structure labels.

- Normal **Aa1-Aa2** code means that the amino acids **Aa1** and **Aa2** linkage belongs to right hand alpha-helix ($\phi = -60$, $\psi = -60$).
- **Aa1~Aa2** code indicates beta-extended (sheet) form ($\phi = -90$, $\psi = +120$).
- **Aa1^Aa2** code indicates reverse beta-turn ($\phi = -90$, $\psi = -30$ are chosen arbitrarily for all the possible versions of reverse turns).

1.1 Amino Acid Shorthand Codes

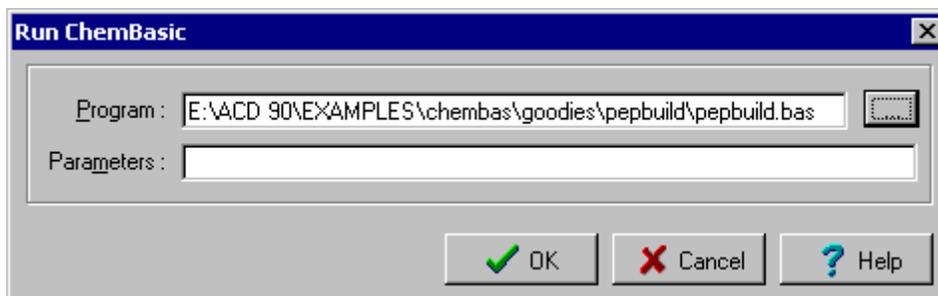
Name	Single letter code	Three letter code
Alanine	A	Ala
Arginine	R	Arg
Asparagine	N	Asn
Aspartic acid	D	Asp
Cysteine	C	Cys
Glutamic acid	E	Glu
Glutamine	Q	Gln
Glycine	G	Gly
Histidine	H	His
Isoleucine	I	Ile
Leucine	L	Leu
Lysine	K	Lys
Methionine	M	Met
Phenylalanine	F	Phe
Proline	P	Pro
Serine	S	Ser
Threonine	T	Thr
Tryptophan	W	Trp
Tyrosine	Y	Tyr
Valine	V	Val
Ornithine ¹	O ²	Orn

¹ Not an amino acid coded for by DNA, but is a central part of the urea cycle.

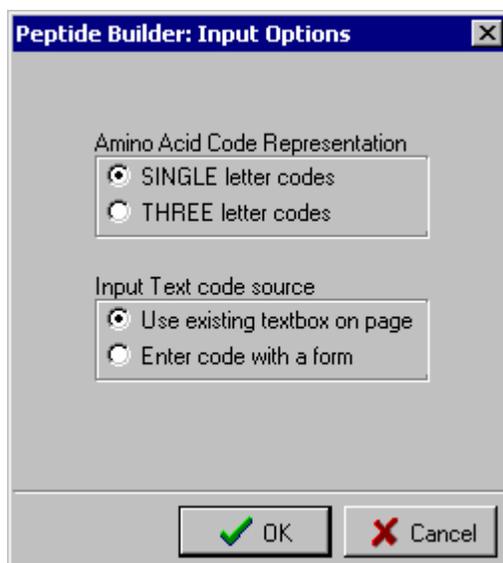
² O is not officially used as a Single letter code.

1.2 Running ACD/Peptide Builder

1. Start the program by clicking **Peptide Builder**  on the ChemBasic toolbar (ChemSketch window) or navigate to the PEPBUILD.BAS file with the **File > Run ChemBasic** menu.



2. A dialog box will appear to allow for the selection of the type of short-hand letter codes to use and how the codes will be entered.



1.2.1 Amino Acid Code Representation

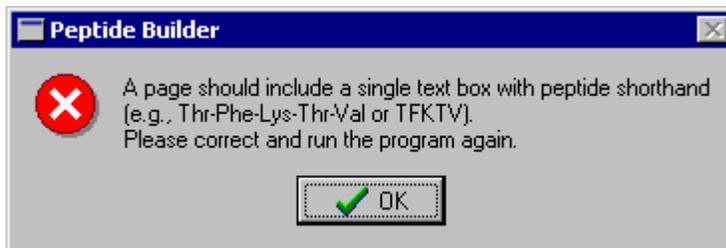
Option	Description
SINGLE letter codes	Use single letter code shorthand, e.g., TAKFTV
THREE letter codes	Use three letter code shorthand, e.g., Thr-Phe-Lys-Ala-Val

1.2.2 Input Text Code Source

Option	Description
Use existing textbox on page	The shorthand code must already exist in a single textbox on the active ChemSketch page. This should be the only textbox on the page.
Enter code with a form	The shorthand code can be entered in a form.

1.2.3 Using an Existing Textbox with the Shorthand Codes

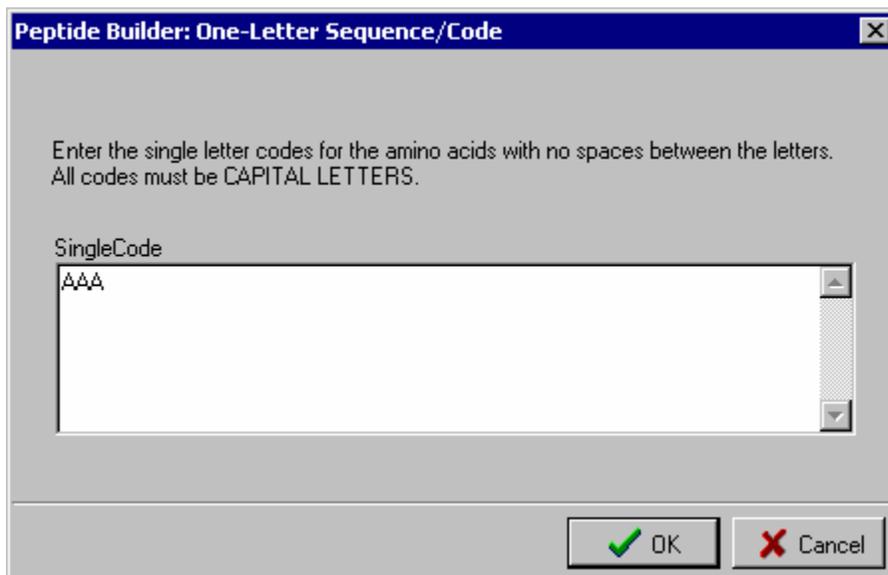
If using the textbox option, you must already have typed in your shorthand code on the active ChemSketch page. If there is no textbox present, you will get the following error message:



1.2.4 Entering Shorthand Code with a Form

If you choose to enter the shorthand code using a form, then one of the following forms will be presented depending on your selection of SINGLE or THREE letter codes.

SINGLE letter code entry form

A dialog box titled "Peptide Builder: One-Letter Sequence/Code" with a close button (X). The text inside says: "Enter the single letter codes for the amino acids with no spaces between the letters. All codes must be CAPITAL LETTERS." Below this is a text input field labeled "SingleCode" containing the text "AAA". At the bottom are "OK" and "Cancel" buttons.

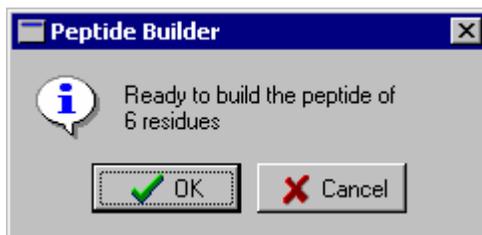
THREE letter code entry form

Once the shorthand code has been entered by either the textbox method or a form, the construction of the peptide is the same. Just follow the instructions in the subsequent dialog boxes that appear.

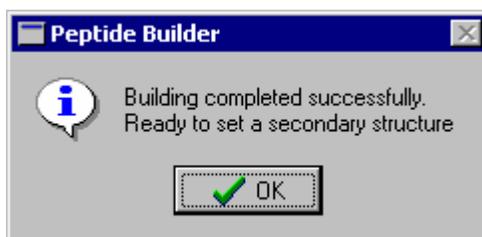
1.3 Example 1. SINGLE Letter Code Input with Textbox

1. Enter the following text on the ChemSketch page: `vLIGSF` (or load the example file PEPBUILD.SK2 and go to page 2.)
2. Run the Peptide builder and choose the options as shown in the dialog box below:

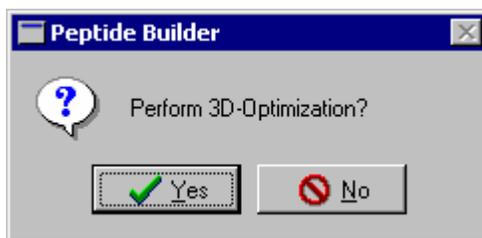
3. The entered code will be checked and then a confirmation dialog box will be presented indicating the number of peptide residues. Click **OK** to continue.



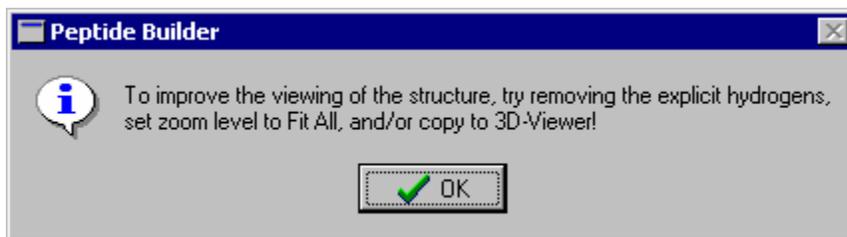
4. A confirmation dialog box will indicate the success of building the primary structure and is now ready to set the secondary.



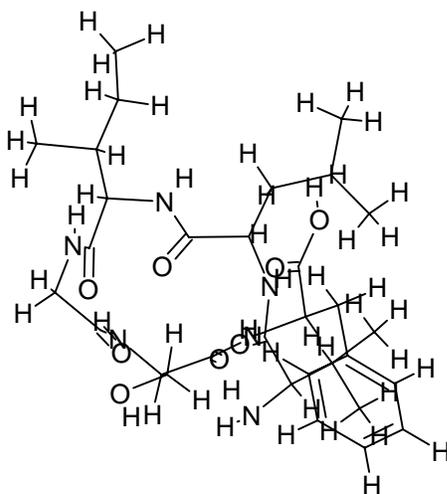
5. You will then be prompted to perform a 3D-Optimization. Depending on the size of the peptide, this may be performed in several stages and can take some time. For this current example click **YES**.



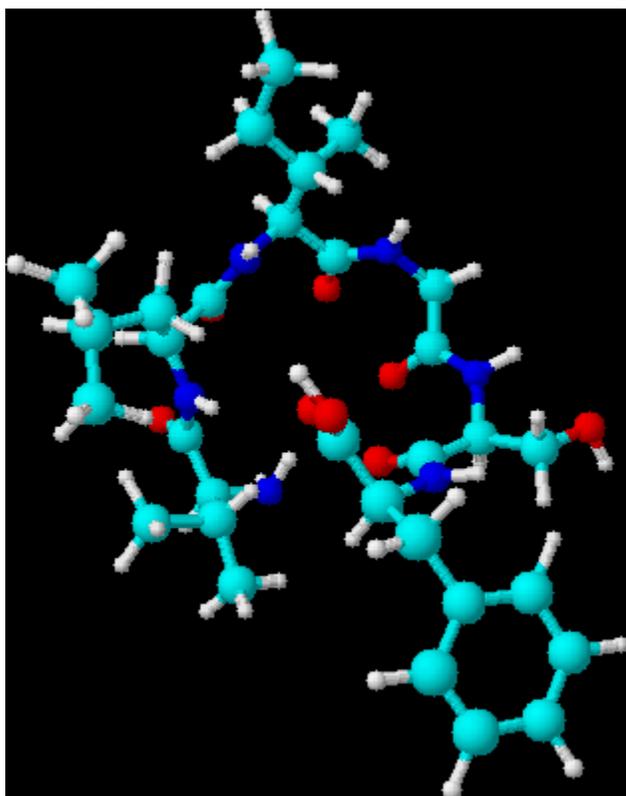
6. When the 3D-Optimization is complete, you should see your structure on the page. A dialog box will make some suggestions on how to best view the structure if it is too large to see with the current ChemSketch window settings.



7. The final structure for **VLIGSF** should look similar to the following image:



8. This structure can then be pushed into the 3D-Viewer for further investigations.



1.4 Example 2: THREE Letter Code Input

Enter the following code either on the THREE letter code entry form or via a textbox in ChemSketch. (This is the same as the example on page 3 of the example file PEPBUILD.SK2).

Trp-Phe-Lys-Ala-Pro-Val-Cys-Trp-Phe-Lys-Ala-Pro-Val-Cys-Trp-Phe-Lys-Ala-Pro-Val-Cys

Follow steps 2–8 as in Example 1 above. The final structure will look similar to the following:

