

# Upgrading Databases to SpecManager 8.20 Format

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## SpecDB Version 8.0

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## Introduction

ACD/Labs introduced a new database format as part of an interim upgrade to the current [SpecManager](#) [1] database (SpecDB) format. This impacts a number of products including [ChromManager](#) [2], [Curve Manager](#) [3], [MS Manager](#) [4], [1D NMR Manager](#) [5], [2D NMR Manager](#) [6], and [UV-IR Manager](#) [7]. The new format will be designated with a new file extension (\*.ND8) to differentiate it from the current databases format (\*.ND5) and earlier versions (\*.NDB). Due to incompatibilities in the data model, it is not possible to update databases of previous versions with the current software. To continue using your current databases, an upgrade procedure needs to be completed. This Technical Note will guide you through this procedure.

## User Data Representation

Starting with version 8.20 of SpecDB, the User Data is split into three different categories:

### Structure User Data

This contains additional information assigned to the current structure. Formula (**Formula**), formula weight (**FW**), structure-based predictions, and other user-defined items will be stored here. Several structures can be stored in a database record.

### Document User Data

This subwindow contains additional information about the current spectrum or chromatogram (collectively referred to as 'Documents'). Information on the document such as Hit Quality Index (Hqi), spectral similarity, and other user-defined items will be stored here. One database record can contain several documents.

### Record User Data

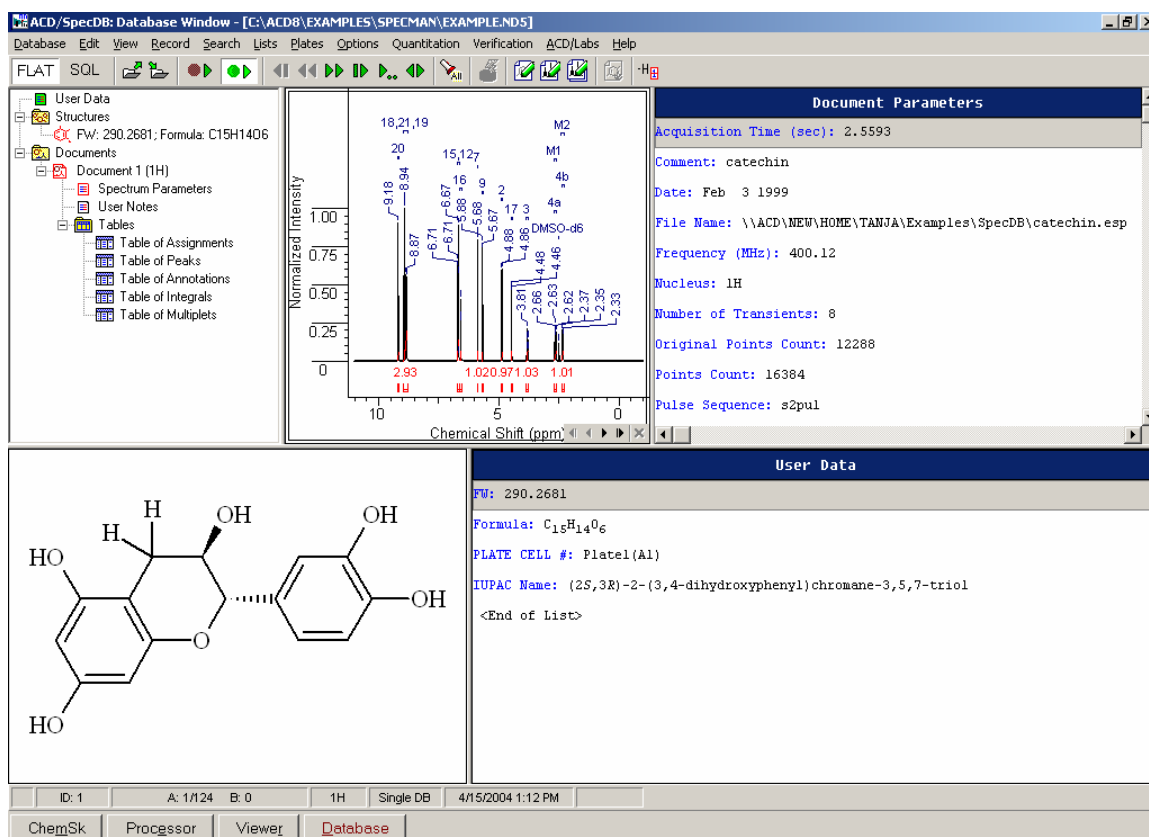
This contains additional user-defined information about the current database record entry.

## Upgrading a Database to SpecManager 8.20 Format

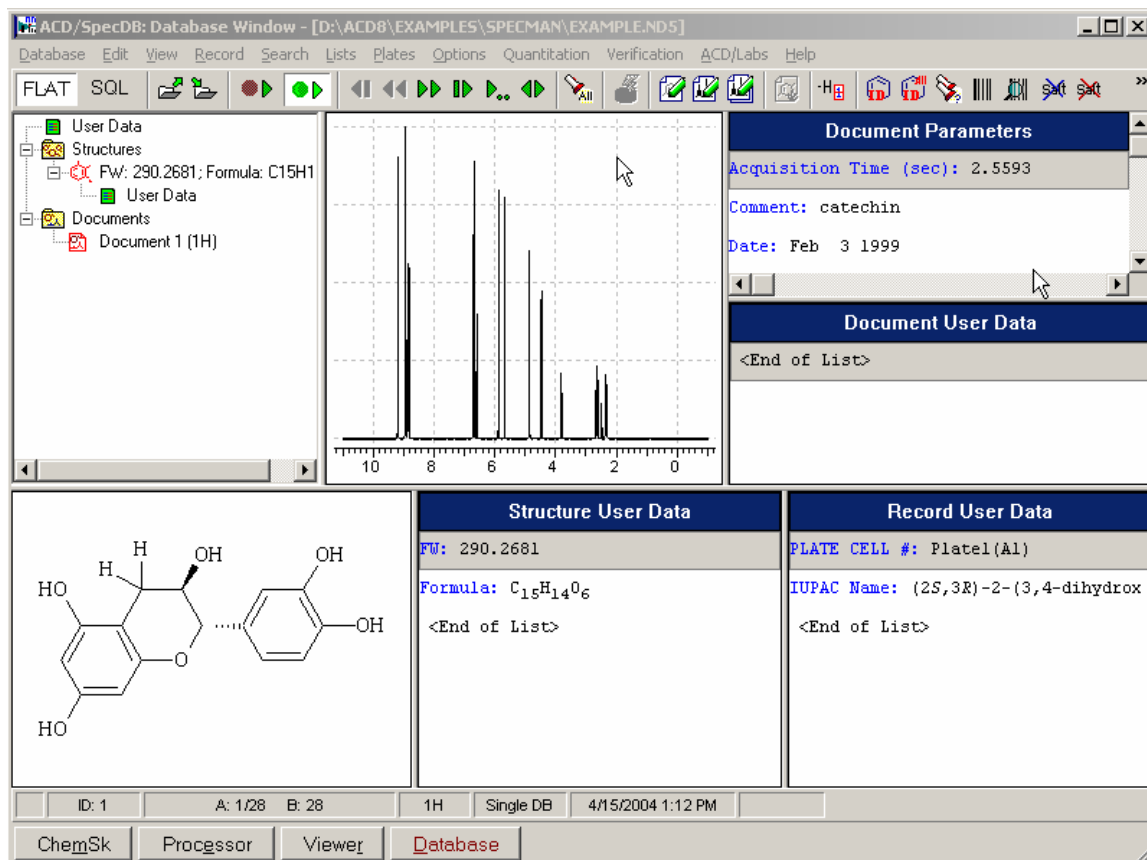
This technical note assumes that you have upgraded your SpecManager software to the latest version by using the Online Updater, your internal update server, or by re-installing your software.

Before continuing, it is imperative that you create a backup of your current database before proceeding. Interruptions or problems may occur during the upgrade procedure that may render your database unreadable in any version of ACD/Labs software. Backups simply involve copying your current database file to a new location. It is recommended that you get advice from your IT professional to implement backup procedures.

1. In this technical note, the EXAMPLE.ND5 file will be used. It is likely located in the ACD8\EXAMPLES\SPECMAN\ folder. Before the upgrade, the Default view of the database displays one subwindow for the User Data Fields:



2. When you launch SpecDB 8.20, note that the default view in v.8.20 now has three different subwindows for User Data.

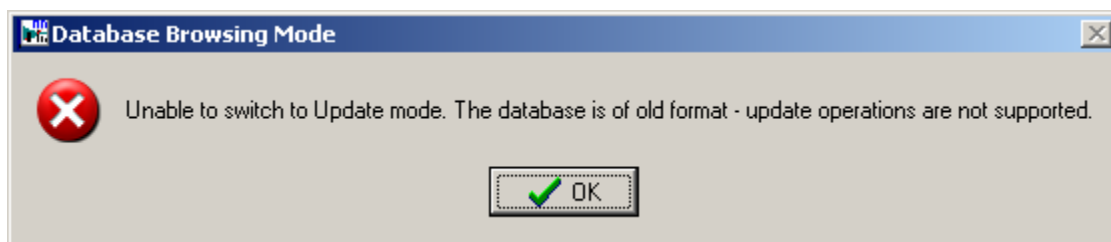


The screenshot shows the ACD/SpecDB Database Window for the file [D:\ACD8\EXAMPLES\SPECMAN\EXAMPLE.ND5]. The interface includes a menu bar (Database, Edit, View, Record, Search, Lists, Plates, Options, Quantitation, Verification, ACD/Labs, Help) and a toolbar with icons for various operations. The main window is divided into several sections:

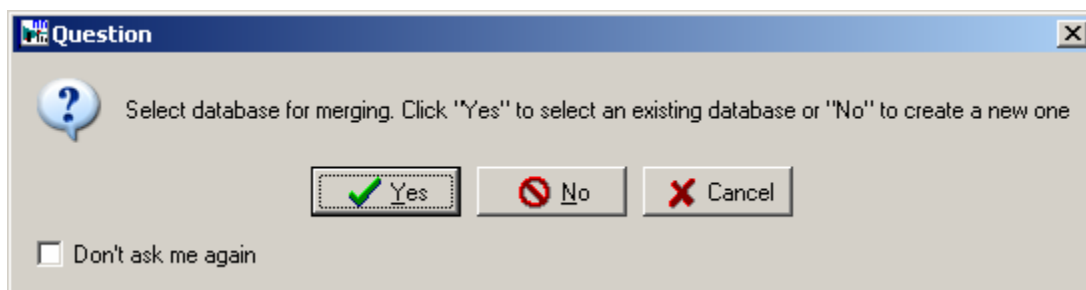
- Left Panel:** A tree view showing the database structure with folders for User Data, Structures, Documents, and Document 1 (1H).
- Center Panel:** An NMR spectrum plot with a chemical structure of catechin overlaid. The x-axis represents chemical shift in ppm, ranging from 10 to 0.
- Right Panel:** Document Parameters and Document User Data sections. The Document Parameters section shows: Acquisition Time (sec): 2.5593, Comment: catechin, and Date: Feb 3 1999. The Document User Data section shows: <End of List>.
- Bottom Left Panel:** A chemical structure of catechin, showing a flavan-3-ol core with multiple hydroxyl groups.
- Bottom Middle Panel:** Structure User Data section showing: FW: 290.2681 and Formula: C<sub>15</sub>H<sub>14</sub>O<sub>6</sub>.
- Bottom Right Panel:** Record User Data section showing: PLATE CELL #: Platel(A1) and IUPAC Name: (2S,3R)-2-(3,4-dihydroxyphenyl)propane-1,3-diol.

At the bottom of the window, there are buttons for ChemSk, Processor, Viewer, and Database. The status bar at the very bottom shows: ID: 1, A: 1/28, B: 28, 1H, Single DB, 4/15/2004 1:12 PM.

- Open the EXAMPLES.ND5 database using the SpecManager 8.20 or later. As soon as the file is open or when you will try to switch to Update mode (**Database** menu / **Update Mode**), you will see the following message:

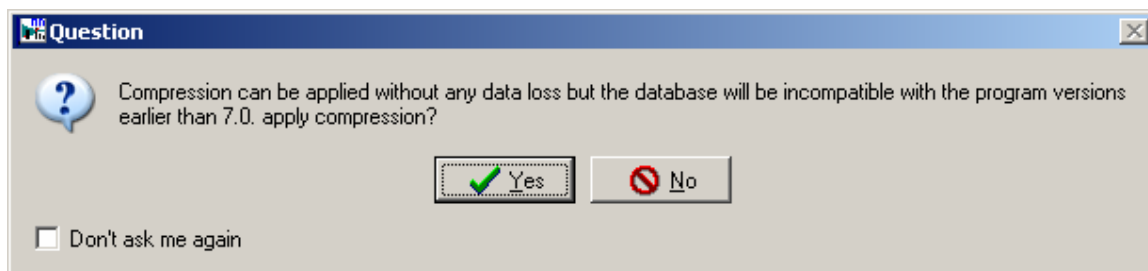


- Click **OK** to work with this database only in Browse mode.
- To be able to update this database, you need to upgrade it to \*.ND8 format. From the **Database** menu select **Tools->Merge to**. A **Question** dialog will appear:



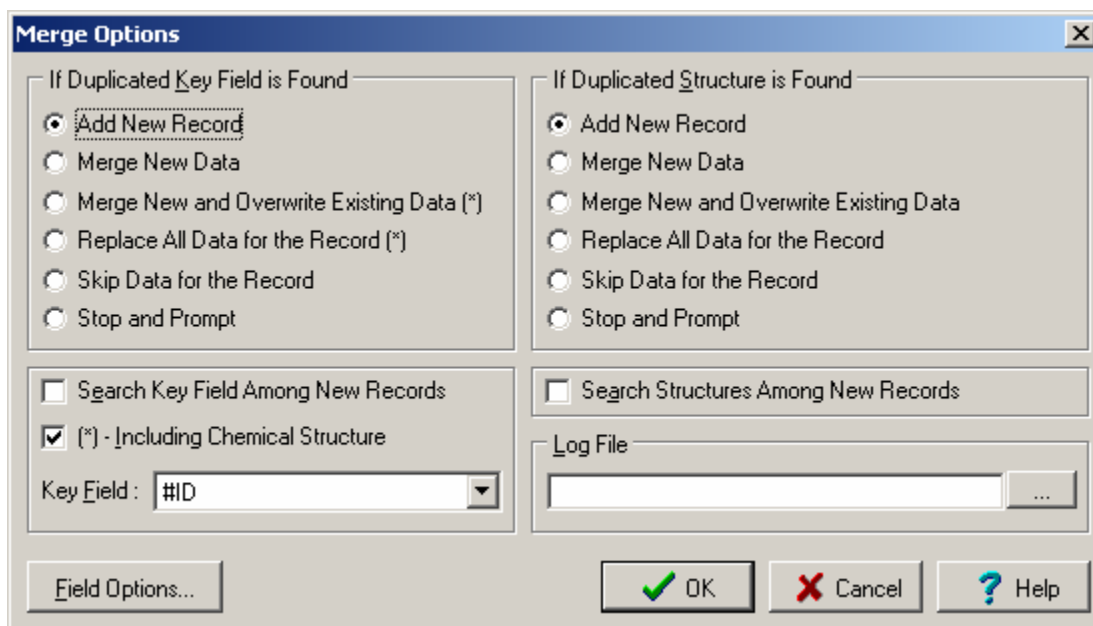
6. Click **No** to create a new database.
7. Specify the name and location of new database and click **Save** in **Create New** dialog box (Test.ND8).

You will see another dialog regarding database compression:



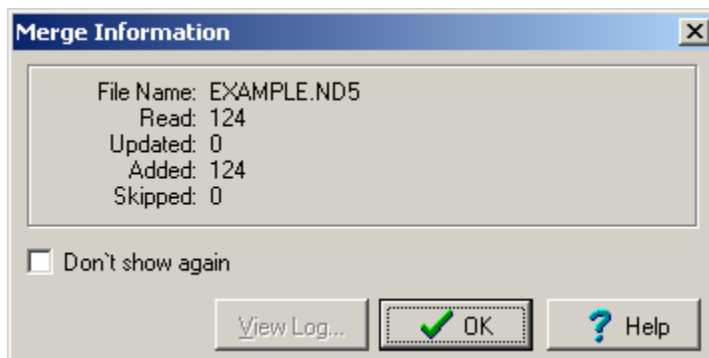
It is recommended that you select "**Yes**" to enable database compression. Compression will reduce the size required to store the database disk space without data loss.

Specify the Merge options in the following dialog box:

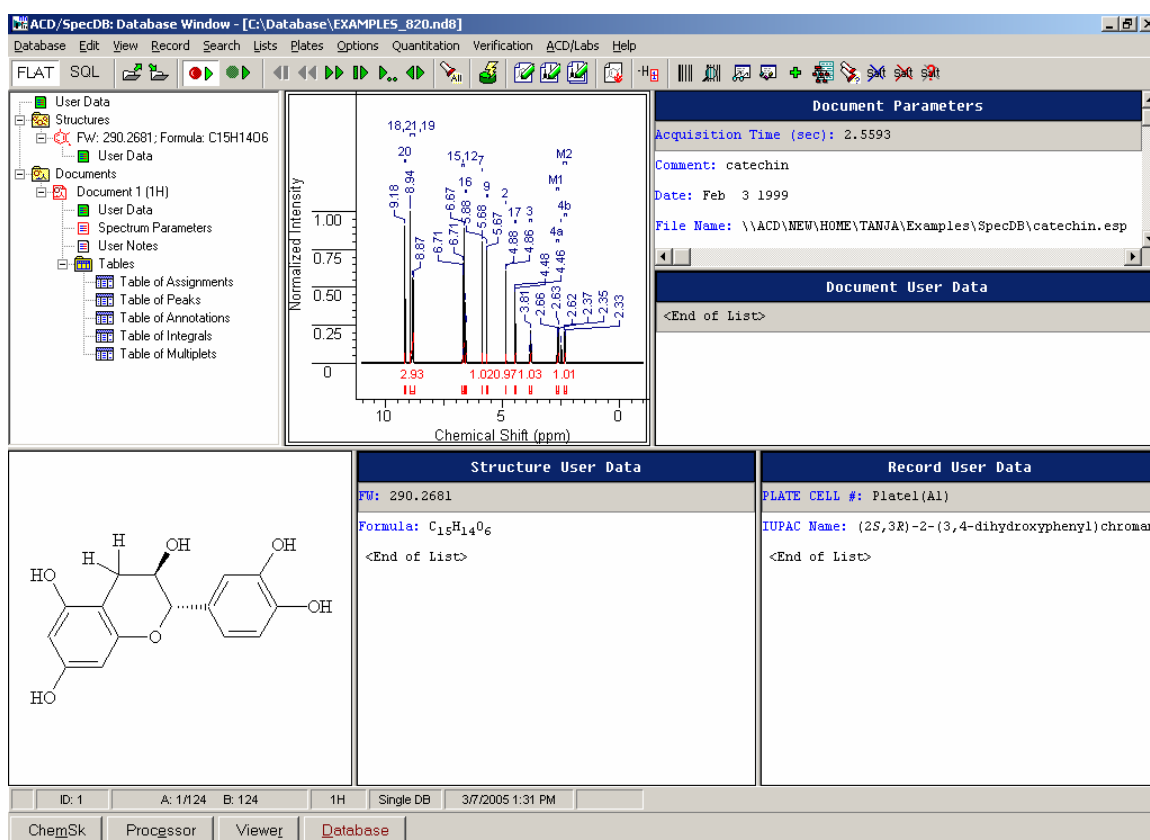


8. Click **OK** to finish the merge.

- After the merge is complete, you will see a summary of all of the actions taken to merge the records. Click **OK** to close this window.



- Open the database you merged to and you will see your database in the new format. You are now able to enter **Update Mode** and add data.



ACD/SpecDB: Database Window - [C:\Database\EXAMPLE5\_820.nd8]

Database Edit View Record Search Lists Plates Options Quantitation Verification ACD/Labs Help

FLAT SQL

Document Parameters

Acquisition Time (sec): 2.5593  
 Comment: catechin  
 Date: Feb 3 1999  
 File Name: \\ACD\NEW\HOME\TANJA\Examples\SpecDB\catechin.esp

Document User Data

<End of List>

Structure User Data

FW: 290.2681  
 Formula: C<sub>15</sub>H<sub>14</sub>O<sub>6</sub>  
 <End of List>

Record User Data

PLATE CELL #: Platel(A1)  
 IUPAC Name: (2S,3R)-2-(3,4-dihydroxyphenyl)chroman  
 <End of List>

ChemSk Processor Viewer Database

## User Data Operations

When you upgrade to the .ND8 format using the **Merge to** function, all the **User Data** will appear in **Record User Data** by default. Formula, FW and all the calculated properties will go to **Structure User Data** by default.

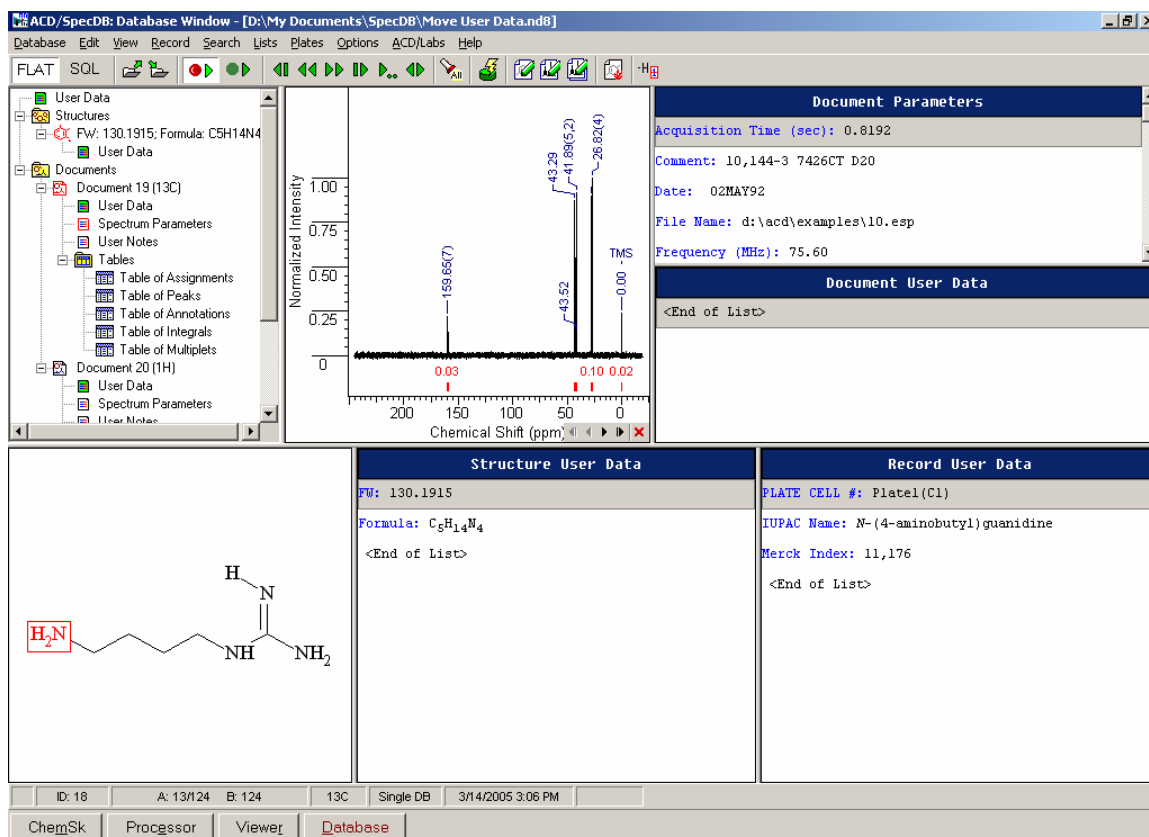
When you update an .ND8 database from the Processor window, a spectrum may have **User Data** and **Structure User Data** already predefined in the processing module. Upon update of the new record, all the fields from **Structure User Data** go to **Structure User Data**; all the fields from **User Data** go to **Document User Data**; and Formula, FW, and all the calculated properties go to **Structure User Data** by default.

When you import an SDF file into a spectral database, all the fields from the SDF file go to **Structure User Data**.

## Moving User Data

Upon importing databases, user data related to structure or spectra will be added to the **Record User Data**. This assignment may not be appropriate for existing **User Data**. To assign existing user data fields to **Structure** and **Document User Data**, a utility has been provided to move existing data fields for all records in the database.

1. Open a SpecManager 8.20 formatted database. In this example we will use the database created from the EXAMPLE.ND5 database.



The screenshot displays the ACD/SpecDB software interface. The main window shows a chemical structure of N-(4-aminobutyl)guanidine, an NMR spectrum with peaks at 159.85(7), 43.29, 41.08(5,2), 43.32, and 26.82(4) ppm, and a table of user data.

Document Parameters	
Acquisition Time (sec):	0.8192
Comment:	10,144-3 7426CT D20
Date:	02MAY92
File Name:	d:\acd\examples\10.esp
Frequency (MHz):	75.60

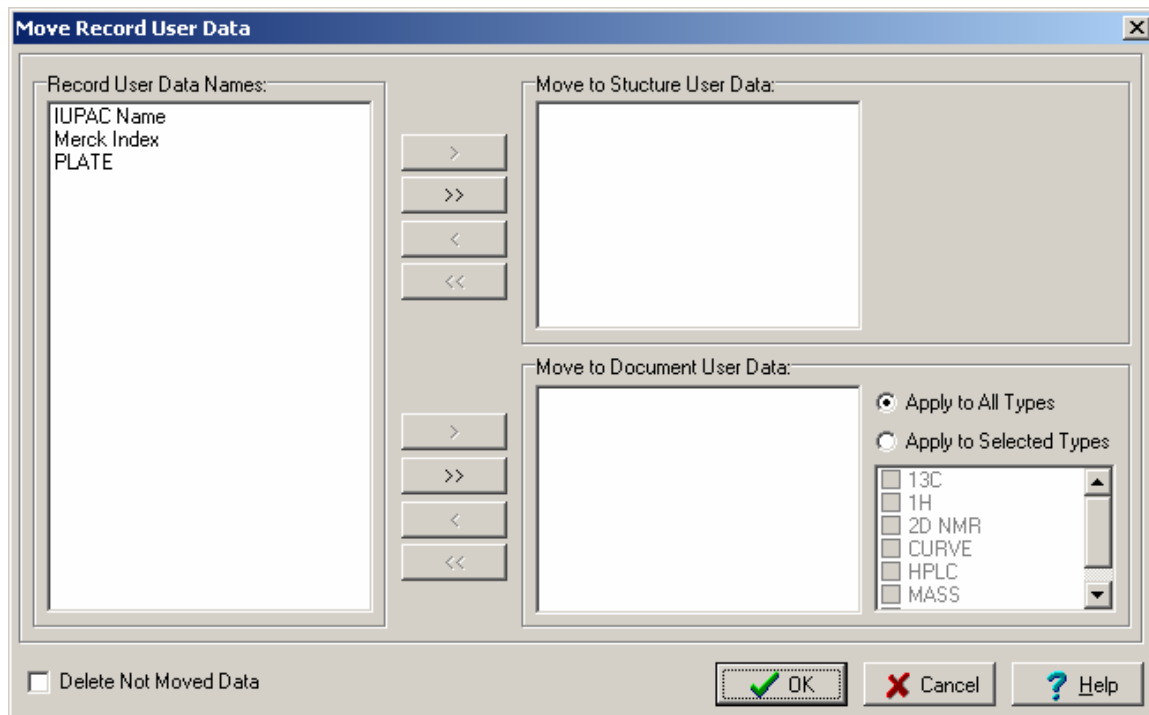
Document User Data	
<End of List>	

Structure User Data	
FW:	130.1915
Formula:	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub>
<End of List>	

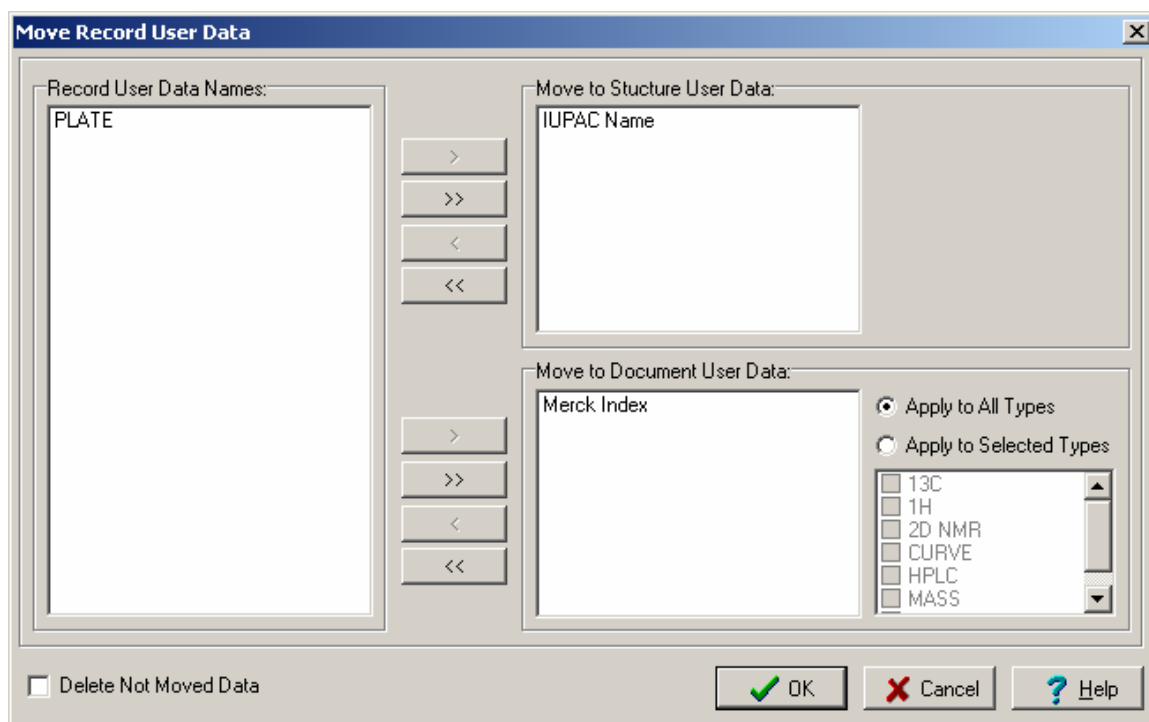
Record User Data	
PLATE CELL #:	Platel(C1)
IUPAC Name:	N-(4-aminobutyl)guanidine
Merck Index:	11,176
<End of List>	

ChemSk Processor Viewer Database

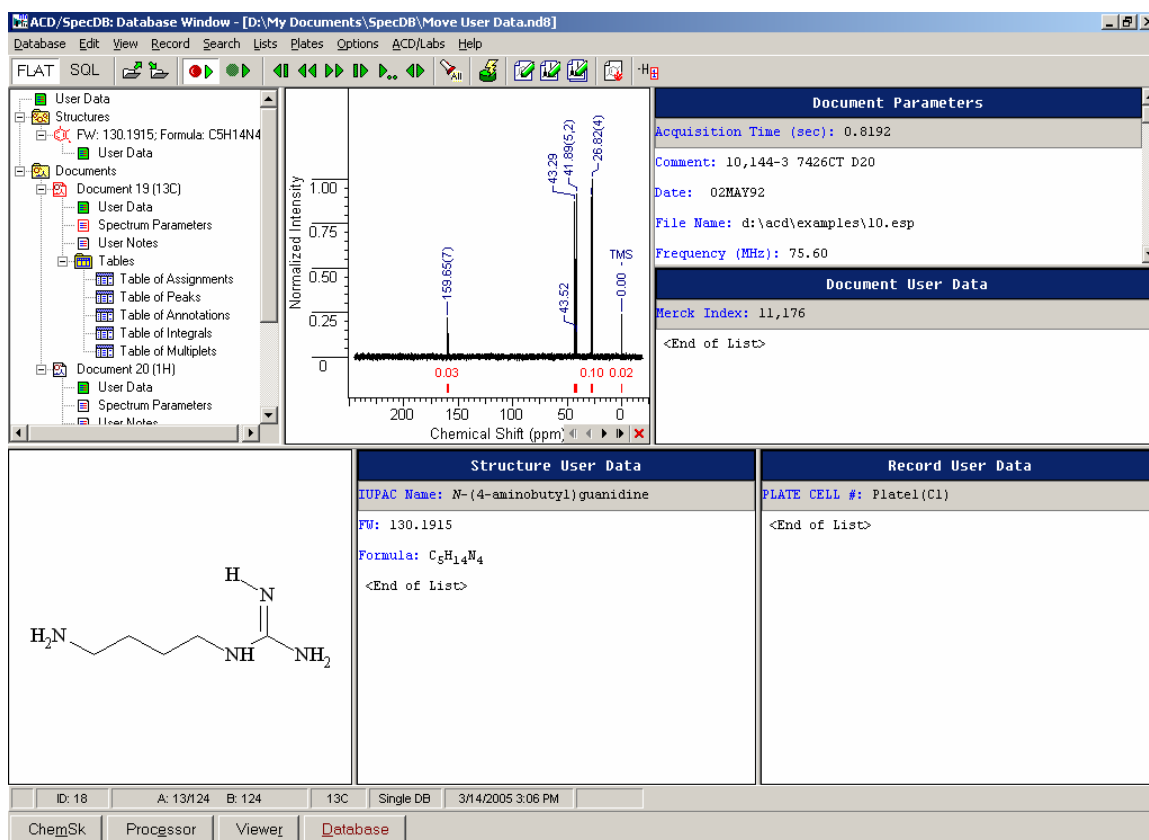
- The user data fields PLATE CELL #, IUPAC Name, and Merck Index have been imported into the **Record User Data**. We would like to move these data fields to the appropriate places on the database. The field: 'IUPAC Name' will be moved to **Structure User Data** and 'Merck Index' to the **Document User Data**. Note that 'PLATE CELL #' is a characteristic for **Record User Data only**—it cannot be moved.
- From the **Database** menu choose **Tools** and point to **Move Record User Data**.
- A new dialog window pops up:



- Select the needed field in **Record User Data Names** and using the appropriate arrows move data fields to **Structure** and **Document User Data**.



6. Please note that the radio buttons **Apply to All Types** and **Apply to Selected Types** allow for added flexibility in assigning **Document User Data** based on spectral method types.
7. An additional check box, **Delete Not Moved Data**, needs special attention. This check box allows you to delete data fields that are not moved.
8. When everything is set according to your data model, click **OK** and the move will be completed within seconds.



## References

1. ACD/SpecManager. [www.acdlabs.com/specmanager/](http://www.acdlabs.com/specmanager/). March 31, 2005
2. ACD/ChromManager. [www.acdlabs.com/chrommanager/](http://www.acdlabs.com/chrommanager/). March 31, 2005
3. ACD/Curve Manager. [www.acdlabs.com/curvemanager/](http://www.acdlabs.com/curvemanager/). March 31, 2005
4. ACD/MS Manager. [www.acdlabs.com/msmanager/](http://www.acdlabs.com/msmanager/). March 31, 2005
5. ACD/1D NMR Manager. [www.acdlabs.com/1dnmrmanager/](http://www.acdlabs.com/1dnmrmanager/). March 31, 2005
6. ACD/2D NMR Manager. [www.acdlabs.com/2dnmrmanager/](http://www.acdlabs.com/2dnmrmanager/). March 31, 2005
7. ACD/UV-IR Manager. [www.acdlabs.com/uvirmanager/](http://www.acdlabs.com/uvirmanager/). March 31, 2005