

Using ACD/SDF Viewer

ACD/ChemSketch and ACD/SDF Viewer Version 10.01

Arvin Moser
Advanced Chemistry Development, Inc.
Toronto, ON, Canada
www.acdlabs.com

Introduction

With Version 10 of ACD/ChemSketch, the option to view SDfiles was introduced into the desktop drawing package via an integrated utility called ACD/SDF Viewer. In this manner, tens of thousands of structures can be viewed within this drawing interface that has become popular with hundreds of thousands of users.

An SDfile (Structure Data File) is a text file containing information about the structure and meta data. The structural information is comprised of x,y,z coordinates and the bond order of bonded atoms. Meta data is comprised of a header followed by a string of data. Typical meta data includes formula weight, formula, *etc.* An SDfile can consist of single or multiple structures.

The benefit of having an SDfile is that it provides a quick and efficient way to move information across a company.

A portion of an SDfile is shown below.

```
7.3615 -3.7543 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0
6.2131 -3.0918 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
6.2131 -1.7594 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
2 3 1 0 0 0 0
> <DSSTox_ID_FileName>
1 CPDBAS_v3b_1481_10Apr2006
```

```
> <STRUCTURE_Formula>
```

```
C11H9N3
```

The advantage of using ACD/SDF Viewer is that you can convert the x,y,z coordinates into a visual representation of the structure and have these structures transferred to both ACD/ChemSketch and ACD/3D Viewer. In addition, the software can quickly search and extract records with specific meta data.

This technical note will illustrate how to use SDF Viewer to view an SDfile and search its contents for pertinent records. In addition, you can modify the interface to graph specific data.

Software Requirements

- ACD/ChemSketch version 10.0 (includes ACD/SDF Viewer and ACD/3D Viewer and other components listed below in Figure 1)
- WinNT, Win2000, or XP operating system

Installing and Loading SDF Viewer

During installation, ensure that the **ACD/SDF Viewer** check box is selected (see Figure 1).

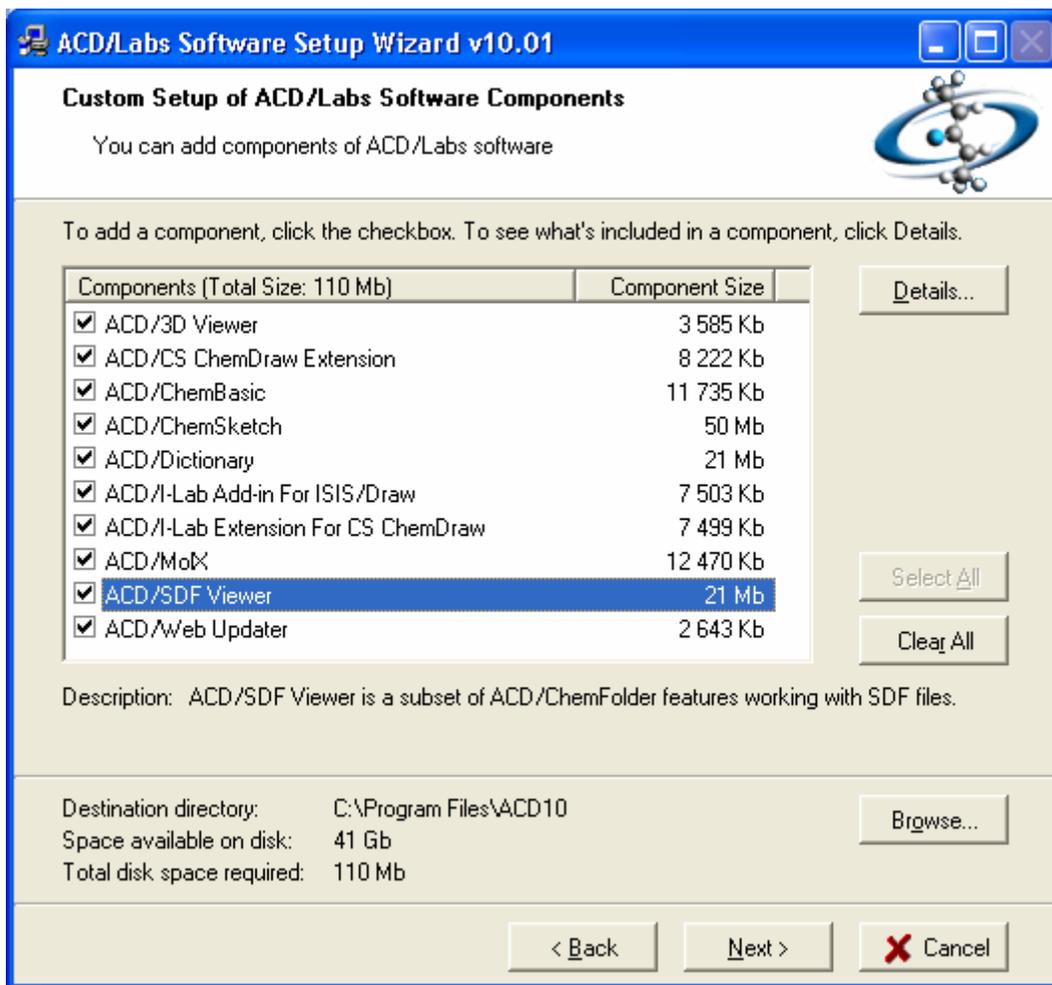


Figure 1: Installation dialog box listing software components. ACD/SDF Viewer is highlighted in blue.

After installation, all ACD/Labs software programs can be accessed from the Start button (click **Start**, point to **Programs**, point to **ACDLABS10**, and then select the software program you want to open; see Figure 2).

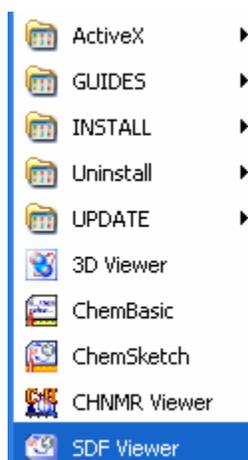


Figure 2: All ACD/Labs software programs can be accessed from the Start button.

Once the ACD/Labs software has been loaded, additional software packages can be accessed from the **ACD/Labs** menu (see Figure 3).

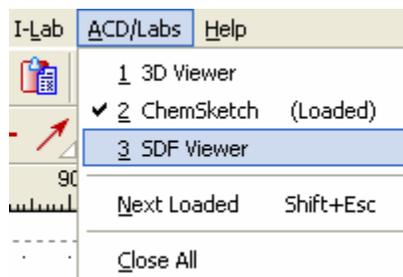


Figure 3: The **ACD/Labs** menu showing access to SDF Viewer and 3D Viewer. The checkmark denotes the active program. Depending on the installation package, additional modules may be present in the list.

Downloading an SDfile from the Internet

Since many SDfiles are available for download from the Internet, this note will demonstrate how to access and view such a file, specifically, Carcinogenic Potency Database Summary Tables—All Species from the U.S. Environmental Protection Agency (Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network). Browse to the website listed below:

<http://www.epa.gov/ncct/dsstox/index.html>

On the right-hand side, select Structure Data Files. Click the link CPDBAS located below the NAMEID column. CPDBAS stands for Carcinogenic Potency Database Summary Tables—All Species, and includes information on Tumor target site incidence, TD50 potencies, summary activity calls for rat, mouse, hamster, dog, and/or non-human primate; data reviewed and compiled from literature and NTP studies.

Click the link **SDF Download Table**. The final screen will show where the SDfile can be downloaded (see Figure 4).

| Data Files: CPDBAS | | | |
|--------------------------------|--|-----------------|---|
| SDF Structure Data File | CPDBAS_v3b_1481_10Apr2006.sdf | |  |
| ▪ Data Table (no structures) | CPDBAS_v3b_1481_10Apr2006_nostructures.xls | *.zip 1916KB |  |
| ▪ Structures Table | CPDBAS_v3b_1481_10Apr2006_structures.pdf (PDF, 30 pp., 3.8 MB) | |  |

Figure 4: The link for the CPDBAS SDfile located at http://www.epa.gov/ncct/dsstox/sdf_cpdbas.html#DownloadTable

Download and unzip the SDfile called CPDBAS_v3b_1481_10Apr2996.sdf.

Loading the SDfile into SDF Viewer

With SDF Viewer loaded, from the **Database** menu, choose **Open**.

Note The **New** command is only available if ACD/ChemFolder is purchased. Browse to the SDfile downloaded in the previous section or to any available SDfile (see Figure 5).

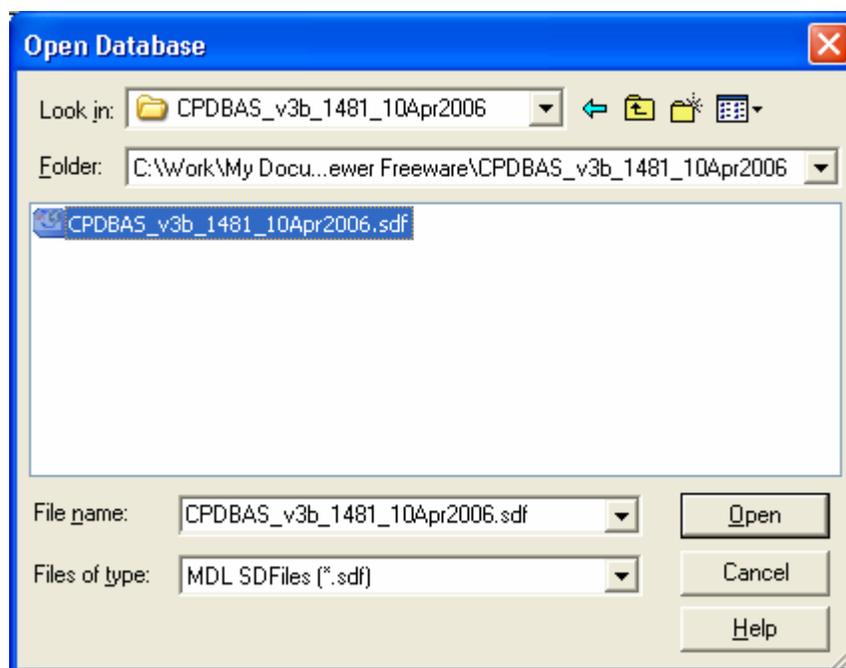


Figure 5: The **Open** dialog box showing the SDfile.

Once the SDfile has been loaded, the current screen will display a structure and meta data as seen in Figure 6. The current SDfile contains 1482 records.

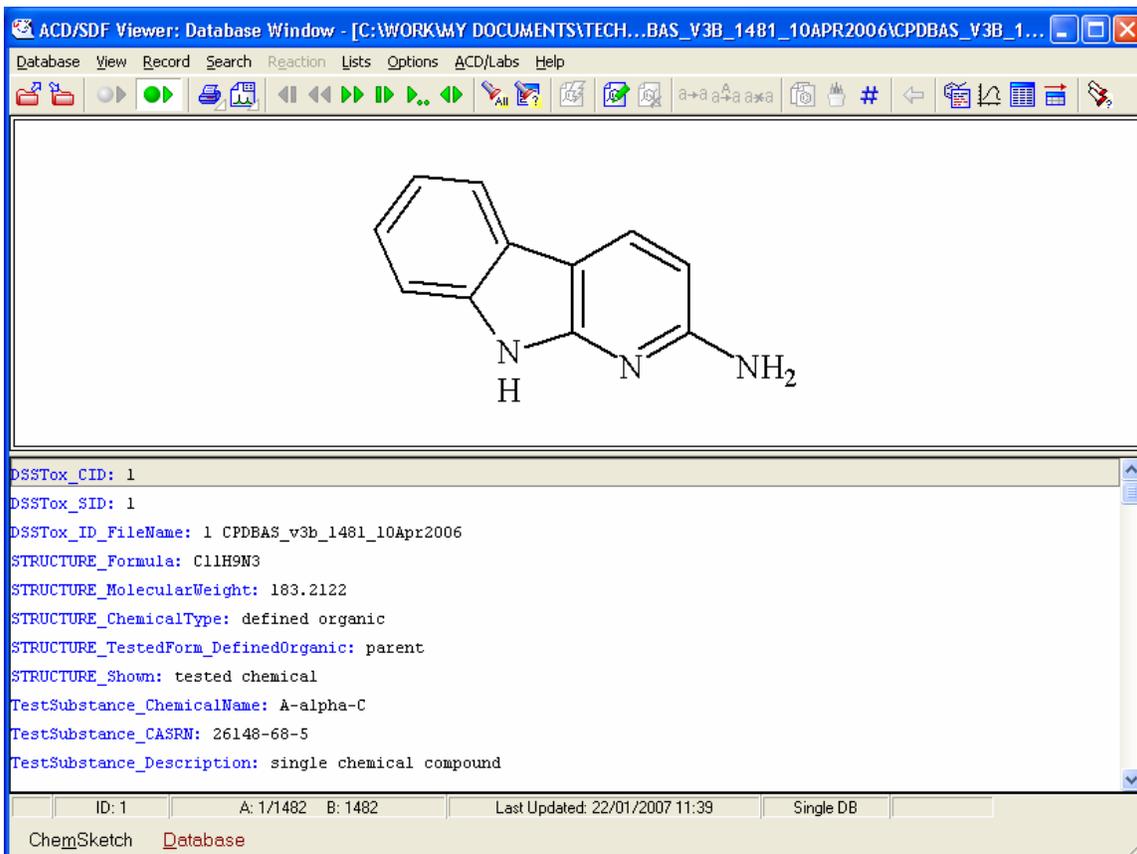


Figure 6: The display for the first record in the SDfile. The total amount of records is listed in List A located near the bottom right corner.

The green arrows located on the toolbar enable you to pan through the various records (see Figure 7).



Figure 7: To pan across the records, use the green arrows located on the toolbar.

To view a group of structures (see Figure 8), from the **View** menu, choose **Tile** (or **Table**). The size of the tiles can be adjusted using the magnifying glass located on the toolbar.

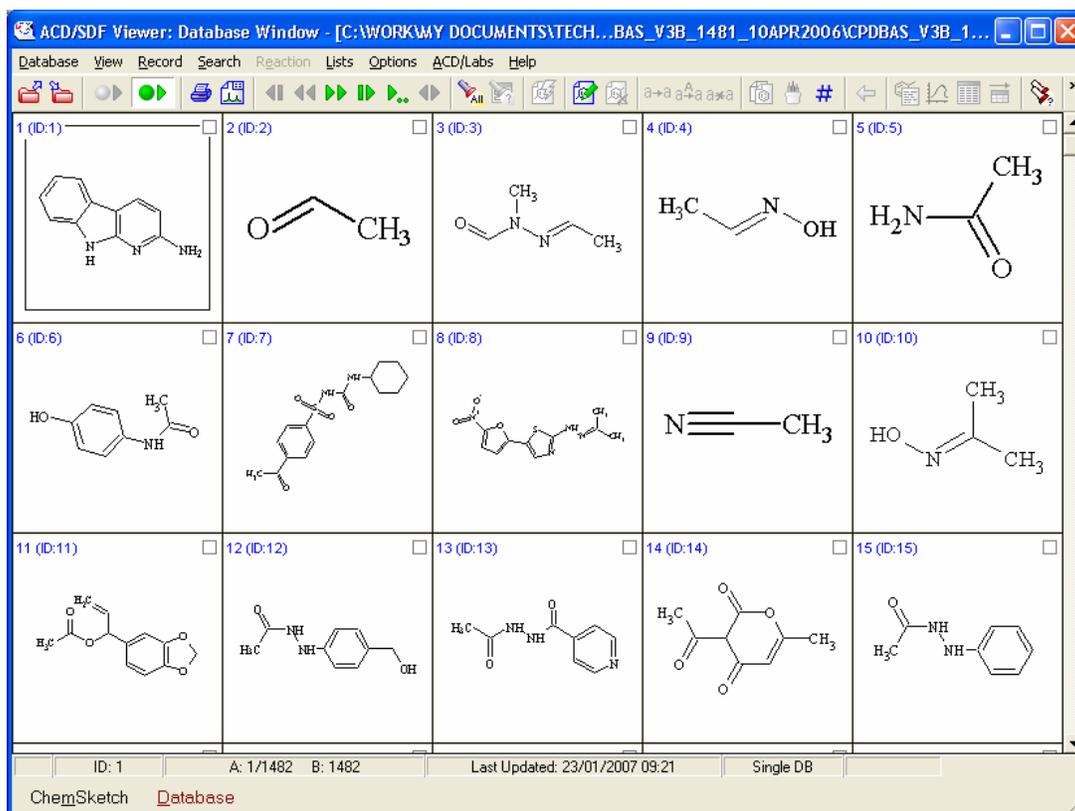


Figure 8: Tile View showing the first 15 structures.

To display meta data beside the structure while in Tile mode, right-click on a structure and select **Select Data**. A **Select Data** dialog box will appear as seen in Figure 9. Select the meta data of interest and push it to the right side.

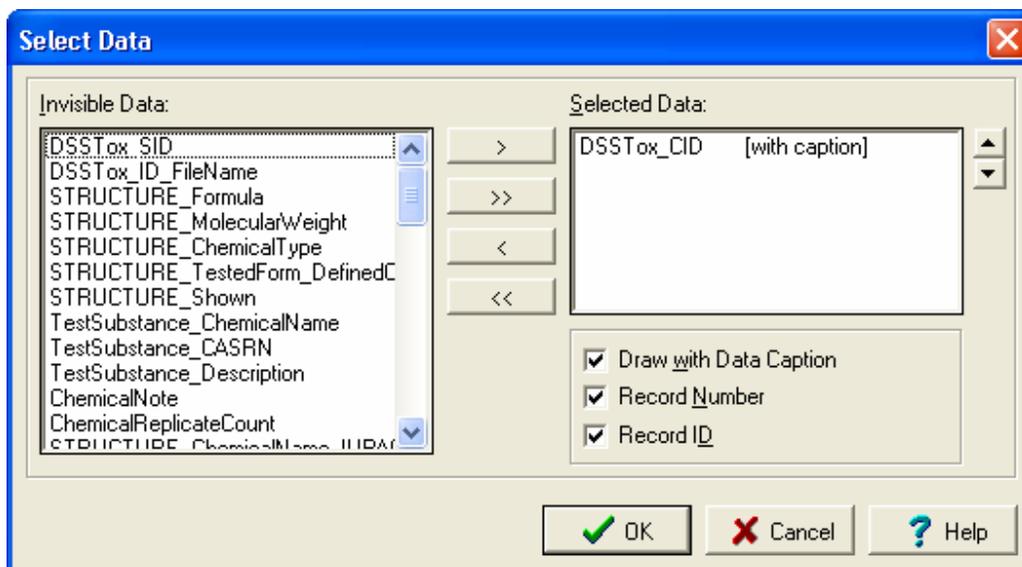


Figure 9: The **Select Data** dialog box listing all meta data available.

Since the **DSSTox_CID** meta data was selected in Figure 9, Tile mode will display it below the structure (see Figure 10).

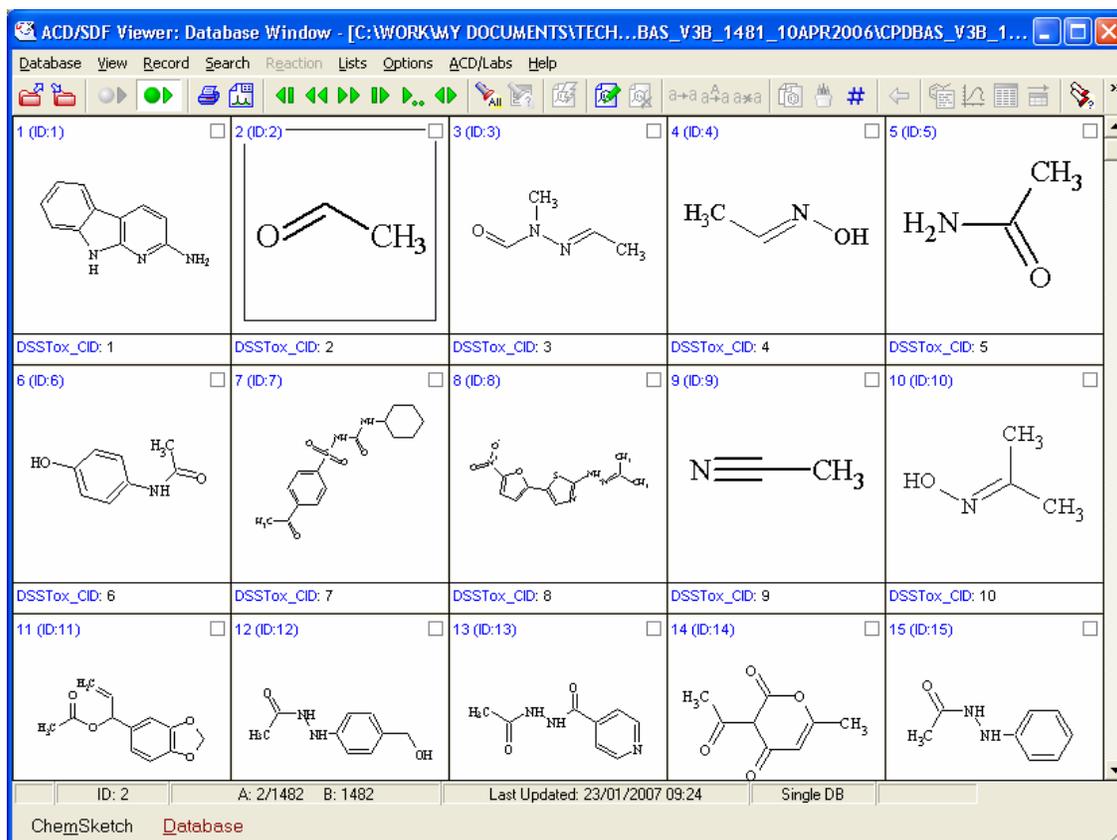


Figure 10: Tile showing the meta data **DSSTox_CID** below each structure. Note that more than one meta data can be shown provided it was set initially.

Searching the SDfile

With the SDfile loaded, various searches are possible, including structure search and meta data search. All Search commands are located under the Search menu. For this example, the meta data will be searched for two conditions.

From the **Search** menu, choose **Data**. Set **Data Names** to *Species Includes mouse*. Then click **More** to add the second condition. Enter the second condition as *ChemicalReplicateCount More Than 1*. Figure 11 illustrates the setup of the dialog box.

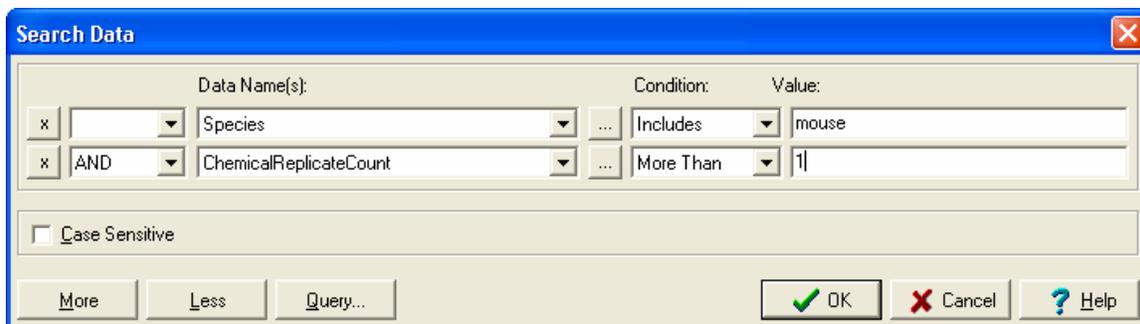


Figure 11: Settings for the **Search Data** dialog box.

Click **OK** in the **Search Data** dialog box. The search results will return 76 hits out of 1482 records.



Figure 12: A dialog box showing the number of hits based on the criteria in Figure 11.

If you would like to search all 1482 records, List A must be reset. From the **Search** menu, choose **Retrieve All**, or click **Retrieve All** .

Designing a User Screen View

The overall view of the interface can be changed to suit your needs. To design a screen view, on the **View** menu, point to **Screen Forms**, and then choose **Edit Screen Form**. To customize the view, select the Data you would like present from the **Select Data Names** dialog box.

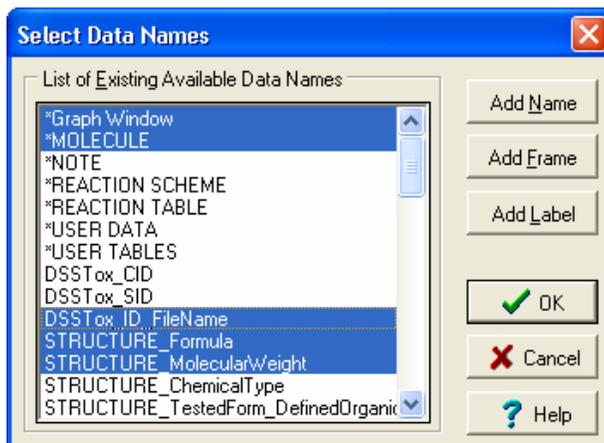


Figure 13: The **Select Data Names** dialog box listing all fields that can be listed. Press and hold **SHIFT** to select multiple Data Names.

Once the Data Names have been selected, resize and reposition the panels to fit the screen (see Figure 14).

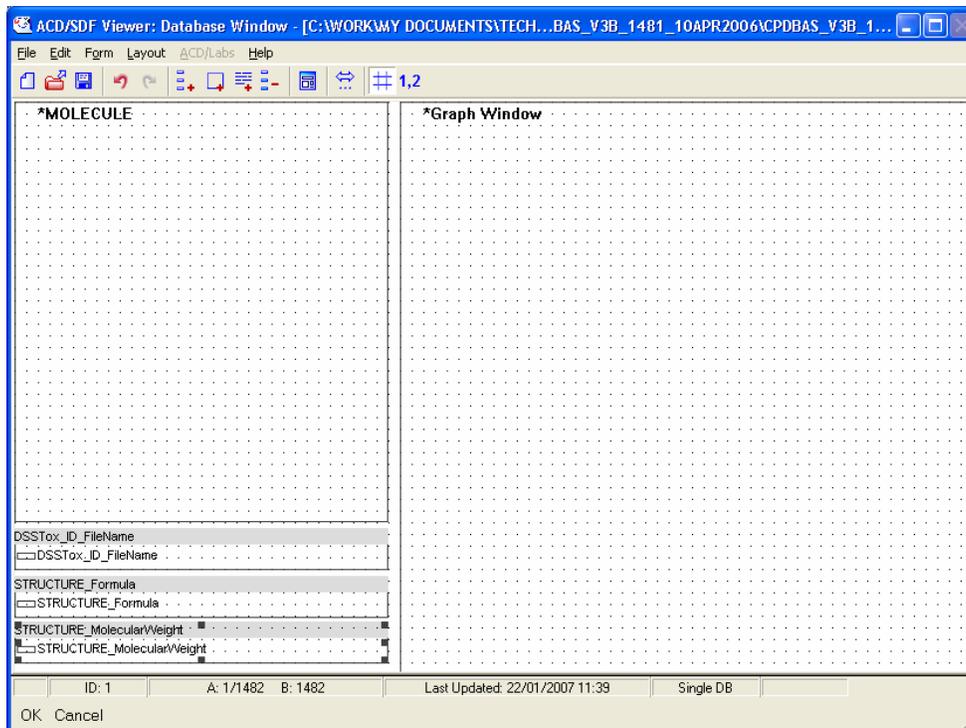


Figure 14: The Data Names were repositioned and resized to accommodate the screen.

Figure 15 illustrates the revamped screen view.

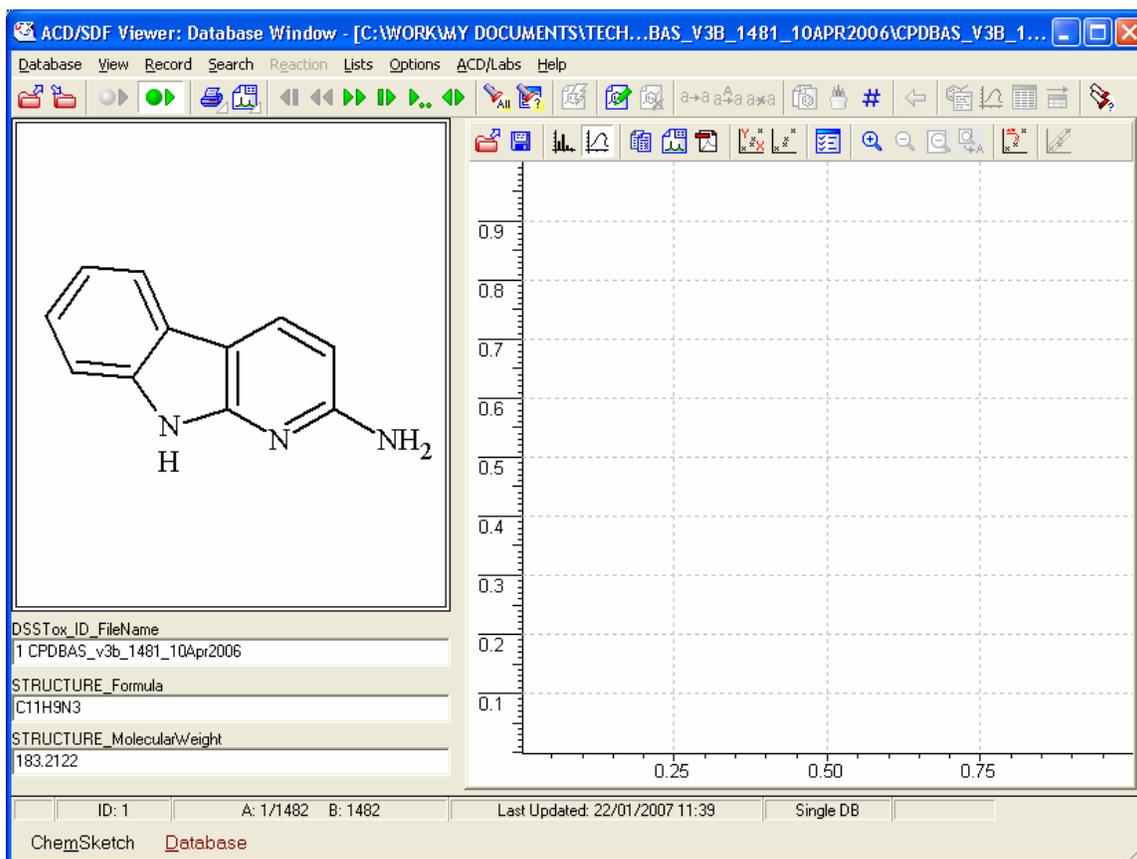


Figure 15: A redesigned screen view showing the structure, 3 specific meta data, and a graph panel.

Graphing Data

Since a graph panel was added from the previous section, this section will demonstrate how to implement a graph based on ID# vs. Molecular Weight. On the Graph toolbar, click **Plot** . The **Select Scatter Plot Data** dialog box will appear as shown in Figure 16.

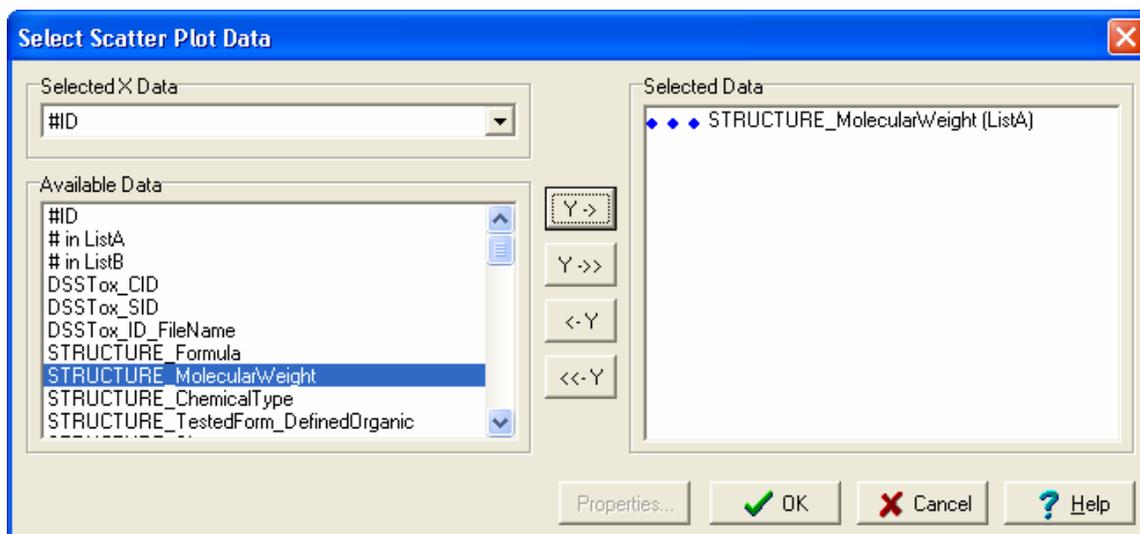


Figure 16: The **Select Scatter Plot Data** dialog box with the X-axis set to #ID and Y-axis set to the meta data Molecular Weight. Note that only records listed in List A will be graphed.

Click **OK** to display the results of the graph (see Figure 17). To view what each spot on the graph is, click on a spot to browse directly to that record. In addition to plotting results, Graph mode can create bar charts, calculate regression results, create reports, etc. All these functions are available on the Graph toolbar.

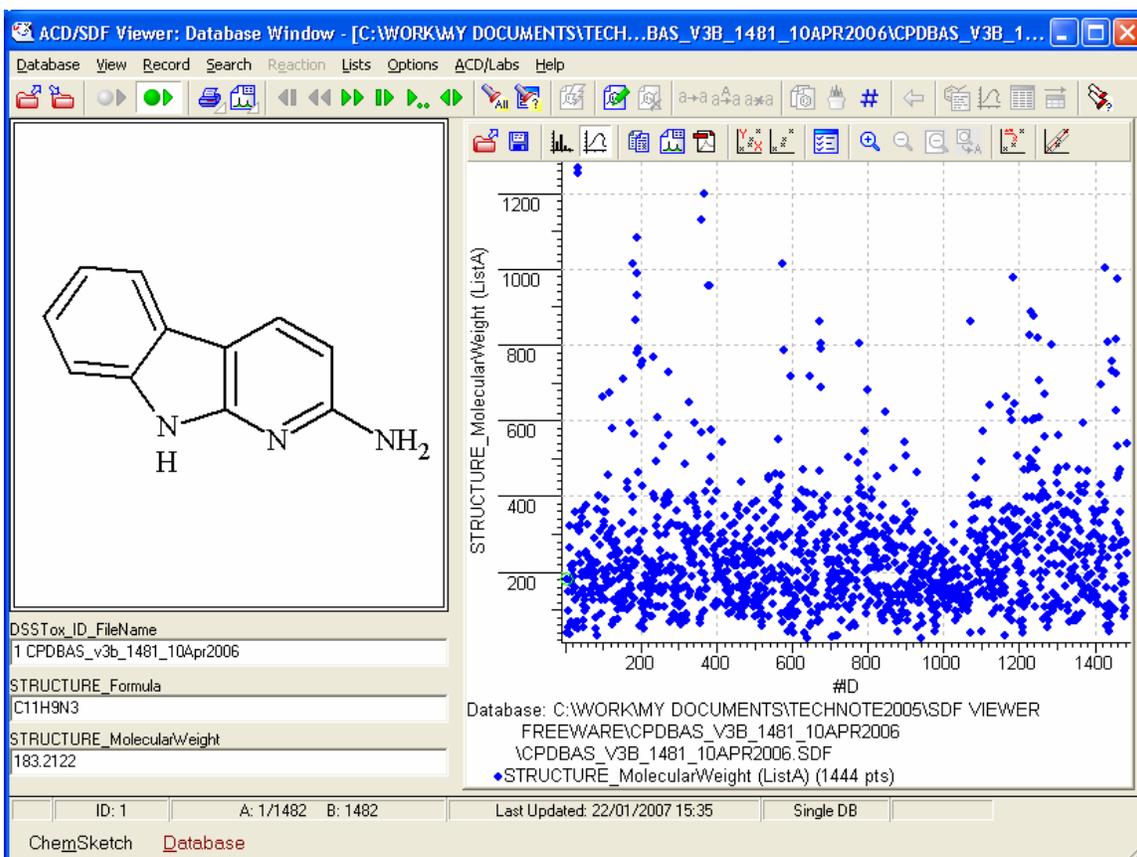


Figure 17: Results are graphed with #ID on the X-axis and Molecular Weight on the Y-axis. Note that only 1444 points out of 1482 were graphed; this is due to some records not containing information on Molecular Weight.

Managing SDfiles with ChemFolder

With the commercial version of ACD/ChemFolder, additional data managing features are available. For example, Import, Merge, and Export SDfiles can be set to check for structure and meta data duplication. Also, searching is significantly faster since the structures are indexed upon converting from the SDF format to the ChemFolder format. For additional information on ChemFolder visit http://www.acdlabs.com/products/chem_dsn_lab/chemfolder/.

Conclusion

ACD/SDF Viewer provides the capability to view SDfiles and to perform multiple searches, all through an easy-to-use interface. The searches are quick and allow you to sift through the data in an efficient manner. For handling SDfiles, the structure drawing package, ACD/ChemSketch, offers the SDfile viewing utility as an added benefit.