



Application Guide

Tips and Tricks using the Accord Settings file

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Introduction

Upon installation of any Accord product, the Accord Chemistry Engine is automatically installed. The Engine is the brains behind Accord's rich chemistry depiction and calculation ability. This set of files includes all of the drivers necessary for Accord to be as diverse and flexible as it is. For Example, files can be imported in virtually any common chemistry file format because the Accord Chemistry Engine provides a driver for each.

The underlying Chemistry Engine allows components and applications, such as the Accord Chemistry Control, Accord Chemistry Cartridge, and Accord for Excel, to seamlessly work together. These components and applications, however, also have their own properties, which can be customized to suit your personal requirements. The Accord Chemistry Engine and many of the components can be configured using the "Accord6.ini" file.

The Accord6.ini file is a text file located at:

```
C:\Program Files\Common Files\Accelrys\Accord 6\System
```

This document will highlight some of the ways that you can optimize and customize certain behaviors or aspects of Accord by manipulating the various sections of this file. However, great care should be used when changing these values and backup versions should always be created and filed away just in case.

1. Optimizing file format handling.

If a file type is not specified during your import or other procedure, Accord will attempt to find the appropriate driver to perform the action by searching a list of available drivers in order from top to bottom. Therefore, if you know that, for example, you commonly read ISIS Sketch 2 files, you can edit this portion of the .ini file to place the ISIS Sketch 2 driver nearer to the top of the list. This placement will speed up performance, since the appropriate driver will be found sooner. Also, if you always use a particular editor, you should move its file format to the top of the list in front of other editor formats.

The top several lines of the file contain the paths to all the Format drivers. It is a good idea to just leave them alone, since having extra drivers will not impact performance.

Amongst the drivers and calculators, there are several sections listing all the available formats to READ, IMPORT, WRITE, etc., such as:

```
[Format: All Read Formats]
```

```
Read=Accord 6.0 Chemistry|Accord 5.0 Chemistry|Accord 6.0 Hex Chemistry|Accord  
5.0 Hex Chemistry|MDL Molfile|MDL Rxnfile|MDL RG Molfile|MDLCT|ChemDraw  
8.x|ChemDraw 6.x|ISIS Sketch 2.x|SMILES|SMD|DARC-F1|CXF|ChemDraw 4.x|ChemDraw  
3.x|Embed Source|ChemDraw Structure Data|Accord 3.1 Chemistry|Accord 3.1  
Hex Chemistry|Accord 3.0 Chemistry|Accord 2.5 Chemistry|Accord 3.0 Hex  
Chemistry|Accord 2.5 Hex Chemistry|ISIS Sketch 1.x
```

This procedure can help when the file format is not specified; however, it is best practice to specify the format whenever possible. Therefore, your SQL statements, for example, should conform to

```
ChemistryMatches( vTarget, vMatchOptions, vQuery [,vFormat][, vOptions][, vLabel] );
```

2. Setting options for reading, writing, importing, & exporting for each file type

You can specify options for certain aspects of how Accord will read or write files, such as fonts to be used if one is not specified:

```
[Format: ISIS Sketch]
WriteOptionsDefault = FontName=Courier
```

Similar entries can be made for specific formatting for particular file export procedures, such as exporting an MDL molfile:

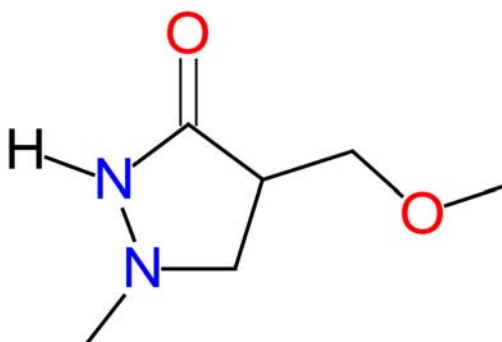
```
[Format: MDL SD Molfile]
ExportOptionsAlways = TrailingZeros=False
```

3. Customizing the depiction of chemical structures

Chemical structures can be displayed with atoms colored differently to make for easier comparison among a set of molecules. You can use the following .ini file entry to designate certain colors to specific atoms. Atoms are identified by atomic number and color using the RGB code (Note the British spelling of Colour).

```
[API Depictor Options]
AtomColour = 7:0,0,255|8:255,0,0
```

The above .ini file entry will make all nitrogen atoms display blue and all oxygen atoms display red.



This option only applies to atom entities. The general syntax is:

```
AtomColour = AtomicNumber1: Red,Green,Blue|=
AtomicNumber2: Red,Green,Blue|...|AtomicNumbern:
Red,Green,Blue
```

'AtomicNumber' should be a valid atomic number from 1 to 109. If zero is specified, the color will apply to special atoms, like element lists, formula nodes, and labels.

To further control how structures are depicted, a new section [API Depictor Options] can be added to the .ini file which may contain the following entries

```
StereoGroupClassChiral = Explicit/All/None
StereoGroupClassGeometric = Explicit/All/None
StereoCategoryLabelChiral = Off/On
StereoCategoryLabelChiralAbsolute = Off/On
StereoCategoryLabelGeometric = Off/On
CIPLabel = Off/On
```

Default values are shown in bold above. These settings can be overridden programmatically by using the Accord SDK functions.

4. Making custom properties available in Accord for Excel

There is a section in the Accord .ini file that controls Accord for Excel, which starts with

```
[Excel]
```

You will see a list of all the user functions and calculators available to you, based on the version of Accord for Excel and any add-on modules you may have installed. They will be listed in two ways: 'DCategory' and 'Category'. 'Category' defines the formula or points to it in the Chemistry Engine, while 'DCategory' displays its name in the Accord for Excel formula list. For example,

```
DCategory ADME Aqueous Solubility=ADME.AQ.SOL.LOG|ADME.AQ.SOL.LOG.LEV|
Category ADME Aqueous Solubility=ADME.AQ.SOL.LOG|ADME.AQ.SOL.LOG.LEV|
```

So to add a custom formula and have it displayed in Accord for Excel, you may enter

```
DCategory MyFunctions=MyNewProperty|MyOtherProperty|Category
MyFunctions=(Chemistry.Weight($$)*2.6) + (ADME.AQ.SOL.LOG.LEV($$)*3.7) - (1.8/
FST.ALOGP98($$)) | (Chemistry.Weight($$)*2.6) + (ADME.AQ.SOL.LOG.LEV($$)*3.7) |
```

5. New for Accord Chemistry Cartridge v 6.2, multi-processor support.

Accord Chemistry Cartridge can be configured to employ multiple threads when performing the atom-by-atom matching phase of a chemistry search via the Accord settings file. Employing multiple threads for processing will result in a faster search by roughly a factor of the number of threads used.

The following entry must be added to the [SDK] section of the Accord6.ini file:

```
jobs=x
```

Where x is the maximum number of threads to be created and used for atom-by-atom matching. For example, adding the following section will configure the atom-by-atom matching phase to employ 2 threads:

```
[SDK]
jobs=2
```

If the multiple thread support entry is not found in the Accord settings file, Accord Chemistry Cartridge employs the default configuration of a single thread. See "Indexing and the search process" on page 5-4 of the Accord Chemistry Cartridge Developer's Guide for details of the available search methods that employ atom-by-atom matching.

6. New for Accord Chemistry Cartridge v 6.2, new terms for improved indexing.

In version 6.2 of the Accord Cartridge, there is a new "Accord Terms 2" format used during index creation. Use of these terms will result in a 20% performance improvement during similarity searching over the standard "Accord Terms". However, if an organization uses Accelrys DataContent databases in ADE2 format, such as CAP or Metabolism, then backward compatibility is required. This is set in the .ini file Accord Terms driver (accordformat12v6.dll) section.

```
similarity=back-compat/6.2
```

The Accord Terms driver section controls whether similarity values are compatible with previous 6.x versions of Accord (back-compat) or whether 6.2 similarity values are produced (6.2).

For a full list of all database, calculator, and format drivers available in Accord, please consult the Accord Chemistry Engine Guide, Chapter 10. Also, new ways to customize Accord using the Settings file continue to emerge with new version releases. It is a good idea to check the Release Notes upon upgrading your Accord application to see if new functionality has been exposed in this manner.