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Experiences Implementing AnIML Viewers and Converters

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Abstract

Introduction to JSpecView and some examples of its use as a web-based viewer.

- sample UV/Vis AnIML document from Stuart Chalk
- JSpecView displaying tartrazine UV/Vis AnIML document
- JSpecView displaying 4-chloroaniline FTIR AnIML document
- JSpecView displaying 1-vinylpyrrolidin-2-one ^{1}H NMR AnIML document

CMLSpec - an alternative XML approach

- JSpecView displaying tetrahydrofuran MS CML document

JSVApp the standalone JAVA application has the ability to read and write files and can be used as a converter.

The strength of Open Source Code is the contributions from others! Volunteer JAVA programmers welcome!
Decompress - conversion of Varian JCAMP-DX NMR files to BLOCK files to Excel
http://usefulchem.blogspot.com/search/label/decompress
http://usefulchem.blogspot.com/2007/01/automated-reaction-kinetics-using.html

JCAMP-DX to AnIML converter by Stuart Chalk
http://fad.coas.unf.edu/animl/jcampconversion2.php

- JCAMP-DX converter at Univ of North Florida

"The Streaming API for XML (StAX) is the latest standard for processing XML in the Java™ language. As a stream-oriented approach, it often proves a better alternative to other methods, such as DOM and SAX, both in terms of performance and usability." from http://www-128.ibm.com/developerworks/library/x-stax1.html

Acknowledgments

ABSTRACT

Free or Open Source spectroscopy viewers are not common. A few exist for specific techniques like IR or NMR but for a wider range of techniques the availability is more limited. Those that do exist are often able to read at least some form of JCAMP-DX file and some can be used to convert between file formats.

JSpecView was released on Sourceforge as Open Source in March 2006. This project was originally intended to provide a JAVA applet and application that would act as a viewer for JCAMP-DX files. The project was later extended so that the viewer could read and write XML documents (both AnIML and CML).

The basic requirement for the viewer in any of these formats is that they contain:

- continuous XY data or
- non-continuous XY data either as a plot or peak table.

At present other formats can not be read or viewed.

The method used for parsing the XML documents is StAX with the JAVA streaming JSR173 API. For writing XML documents the procedure has been to create templates for use with Velocity.

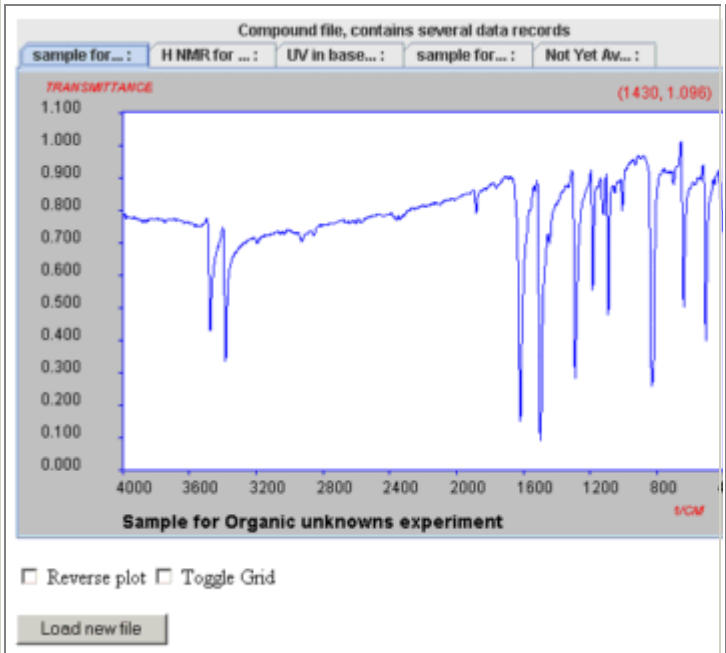
During the initial implementation some of the schemas had not reached the current level of stability. When changes were made that affected the conversion of say a JCAMP-DX file to an AnIML document it was simply a matter of changing the template rather than having to change the JAVA source code. Since all the AnIML documents I have used have been prototypes, any changes in document element names or to the syntax still require re-editing not only all the spectral files but also the JAVA routines used for reading the updated documents.

Some examples of the use of the viewer and as a converter will be highlighted during the presentation.

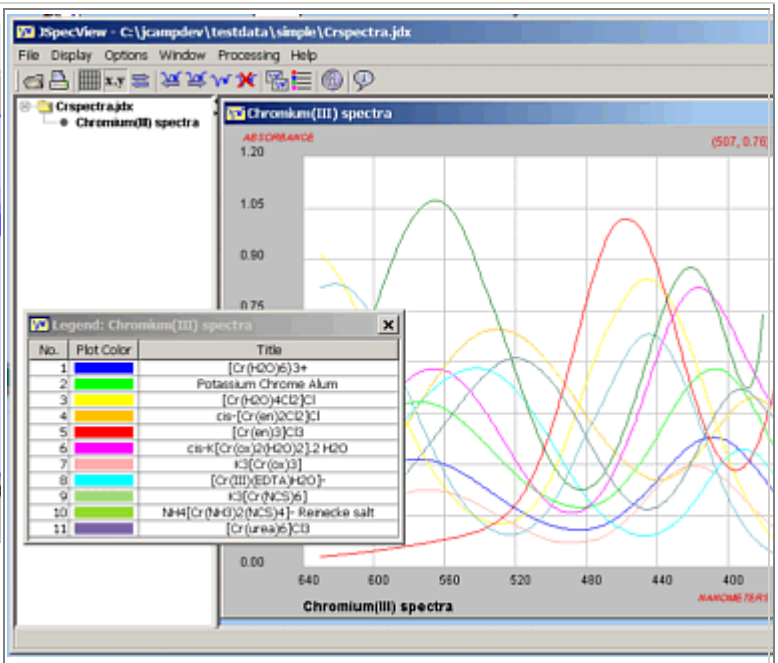
.:. JSpecView Applet Specification

.:. Description

JSpecView is a viewer for spectral data in the JCAMP-DX format. The program was developed at the Department of Chemistry of the University of the West Indies, Mona, Jamaica, WI and is being released via SOURCEFORGE.net under the GNU Lesser General Public License. It is written in JAVA and requires at least JAVA 1.5.



jspecview applet view



jspecview application view

.:. Features

- Load any data file in JCAMP-DX format (limited support for beta vs 6 and importing AnIML and CML files)
- Highlight portions of the spectrum
- Many levels of zooming in and out
- Print the Spectrum
- Reverse the plot
- Show a grid
- Show the coordinates as the mouse moves over the plot
- Convert between Absorbance and Transmittance (for UV/Vis and IR)
- Integrate H NMR spectra
- Has four possible views or interfaces for compound files: single, overlay, tab or tile
- View the header or properties of the spectrum
- Java scripting and Live Connect support *
- Export different JCAMP-DX compression formats *
- Export as AnIML, CML, JPG, PNG or SVG *

* Applets do not normally have permission to write to the hard disk so these functions will not work unless the appropriate permissions are set. In the future JSpecView may be signed and so avoid this problem.

.:. Example web pages using JSpecView, for those who can't wait...

Examples of the applet and web page coding:

- sample 1 load JDX and set plotcolor,
- sample 1b import AnIML and set plotcolor,
- sample 1c import CML and set plotcolor,
- sample 2 load BLOCK file with TABS,
- sample 3 load BLOCK file with radio buttons to select a BLOCK
- sample 4 load BLOCK file with all spectra overlaid.

The use of JSpecView with MDL Chime, Jmol and Marvin can best be seen with some examples....

1. IR spectra and displays of vibrational modes
2. GCMS hotlinked chromatograms
3. MS spectra and animations of fragmentations
4. NMR spectra and displays of links to molecular structure
5. Combination of displays

.:. Parameters

All parameters are passed to the applet as a semi-colon separated list using a **script** call.
The accepted parameters in the list and their description follows:

- **load** To open a spectrum, the name of the JCAMP-DX file must be given. Note that the file must be in the class path of the applet or the full path to the file given.
  The forward slash can be used as a path separator '/' or else escape the backslash using a double backslash '\\'. **This is the only parameter that is required.**
  for example *load filename.dx;* or *load c:/jcamp-dx/filename.dx;* or *load c:\\jcamp-dx\\filename.dx;*
- **import** To import a spectrum stored in AnIML or CML format. Note that the file must be in the class path of the applet or the full path to the file given.
  for example *import filename.aml;* or *import c:/XML/filename.aml;* or *import c:\\XML\\filename.aml;*
  If the extension is .aml or .xml the file is treated as AnIML, if it is cml then the file is expected to be in cml format.
- **gridon** Specifies whether the grid should be displayed
  true or false
- **coordinateson** Specifies whether the coordinates should be displayed
  true or false
- **reverseplot** Specifies whether the plot should be displayed with scale reversed. (This is the reverse of the order of the points in the file)
  true or false
- **startindex** Used along with *endindex* to display only a segment of the spectrum. *startindex* is the index of the staring data point of the segment that should be displayed. If this is specified and *endindex* isn't then a

segment starting from *startindex* to the last data point is displayed.
0,1,2,3...

- **endindex** the index of the last data point of the spectrum to be displayed.
  for example 32765
- **menuon** Specifies whether the menus should be displayed.
  If this is set to **false** then only the ***About*** menu is enabled. This means that zooming is disabled as well.
  To enable zoom, set *enablezoom* **true**.
- **compoundmenuon** Specifies whether the menu that enables the user to choose which spectrum to display (in **single** *interface* mode) is enabled.
  true or false
- **enablezoom** Specifies whether zooming is enabled. Enabling zoom effectively enables the zoom menu and vice versa.
  true or false
- **spectrumnumber** For Ntuple and Block files, this specifies the spectrum that should be initially displayed when the applet is loaded.
  1,2,3...
- **interface** This parameter applies to Ntuple or Block files only. This changes the GUI (Graphical User Interface) of the applet.
  single One spectrum is displayed (default is spectrum number 1). A Ntuple or Block menu is added to the popup menu to navigate to the other spectra in the file.
  tab All spectra are displayed and may be navigated with tabs
  tile A maximum of 10 spectra are displayed and tiled. If there are more than 10 spectra in the file then the interface defaults to **single**.
  overlay The spectra are displayed overlaid.
  single, tab, tile, overlay
- **coordcallbackfunctionname** If this is provided, the applet calls a javascript function by this name and passes it the x and y coordinates of the point on the display that is clicked. Effectively this is a way for the user to provide an action that is to be carried out when the applet or certain points on the applet is clicked.
  (*) a string, e.g. MyCoordCallBack, default null
- **peakcallbackfunctionname** If this is provided, the applet calls a javascript function by this name and passes to it not only the x and y coordinates of the point on the display that is clicked but the closest actual data point and the spectrumnumber (0 if a single spectrum or the block number if a compound or Ntuple file). Effectively this is a way for the user to provide an action that is to be carried out when the applet or certain points on the applet are clicked.
  (*) a string, e.g. MyPeakCallBack, default null
- **titlecolor** The color of the title. All Colors must be specified by an rgb value or as a hexadecimal value. eg. black would be "0, 0, 0" or "#000000". Note that the # is required for hexadecimal format and rgb values must be comma separated.
  default is black (#000000)
- **gridcolor** The color of the grid
  default is grey (#808080)
- **unitscolor**The color of the units
  default is red (#FF0000)
- **scalecolor** The color of the scale
  default is black (#000000)
- **coordinatescolor** The color of the coordinates
  default is red (#FF0000)
- **plotareacolor** The color of the plot area
  default is white (#FFFFFF)
- **plotcolor** The color of the plot line
  (NB. When spectra are overlaid, the first eight colors are: blue, green, yellow, orange, red, magenta, pink and cyan. After that the colors are chosen at random.)
  default is blue (#0000FF)

- **backgroundcolor** The color of the background
  default is grey (#808080)

.:. Scripting and Live Connect

Certain methods in the applet may be called from JavaScript.
These are:

Method	Arguments or Return Values	Description
setFilePath	for example *c:/jcamp-dx/filename.dx* or *c:\\jcamp-dx\\filename.dx*	Allows the loading of a new JCAMP-DX file, specified from JavaScript. Note that the file must be in the class path of the applet or the full path given. The forward slash can be used as a path separator '/' or else escape the backslash using a double backslash '\\'.
getCoordinate	returns space separated values, e.g. "3220 0.41".	Used to return the coordinates of a point when it is clicked on the applet display
toggleGrid	none	Toggles the grid on/off
toggleCoordinate	none	Toggles the x,y coordinate display
reversePlot	none	Reverses the plot
setSpectrumNumber	1, 2, ...	For Ntuple and Block files, this specifies the spectrum that should be displayed.
addHighlight	***x1*** - starting x coordinate ***x2*** - ending x coordinate ***r*** - red value of rgb color scheme. Number from 0-255 ***g*** - green value ***b*** - blue value ***a*** - alpha value or transparency. Number from 0 - 255	Add a highlight to the region specified by x1 and x2 with the color and transparency specified by r, g, b and a.
removeHighlight	***x1*** - starting x coordinate ***x2*** - ending x coordinate	Removes the highlight at the position specified by x1 and x2. There must be a highlight specified by x1 and x2 exactly for this method to work.
removeAllHighlights	none	Removes all highlights from the display.

JSpecView may call a JavaScript function in response to mouse clicks in the plot area of the spectrum display if the **coordcallbackfunctionname** parameter (*) is specified. This function gets passed the values of the x and y position as two floating point numbers. Therefore, a JavaScript function must be implemented with the name given by **coordcallbackfunctionname** and take as its argument two floating point values for the x and y coordinates. Eg. if the value of the **coordcallbackfunctionname** parameter is `onCoordClicked` then a JavaScript method might look like this..

```
function onCoordClicked(x, y){
    alert("You Clicked: " + x + ", " + y);
}
```

Similarly JSpecView may call a JavaScript function in response to mouse clicks in the plot area of the spectrum display if the **peakcallbackfunctionname** parameter is specified. As with the coordcallback function this gets passed the values of the x and y position as two floating point numbers. In addition though it returns the closest actual X,Y values from the dataset and the value of the spectrum number if a Block or Ntuple file is open. Therefore, a JavaScript function must be implemented with the name given by **peakcallbackfunctionname** and take as its argument four floating point values for the two sets of x and y coordinates and an integer for the spectrum number. Eg. if the value of the **peakcallbackfunctionname** parameter is `MyPeakClicked` then a JavaScript method might look like this..

```
function MyPeakClicked(x1, y2, x2, y2, SNum){
    alert("You Clicked: " + x1 + ", " + y1);
    alert("The nearest datapoint was at : " + x2 + ", " + y2);

}
```

Sign up for the users mailing list to get further information and contribute to the discussion.

To download the jar files or source code, visit the Sourceforge Project Page.

Created 1st March 2006. Links checked and/or last modified 13th February 2007.
For further information contact Prof. R.J. Lancashire, Department of Chemistry, UWI, Mona, Kingston 7, JAMAICA, (robert.lancashire@uwimona.edu.jm)

SAMPLE AnIML file courtesy of Stuart Chalk.

```
<?xml version="1.0" encoding="UTF-8" ?>
- <!--
 Example AnIML UV/Vis data file to show the development of the UV/Vis technique definition
 -->
   - <!--
    Using schema

        * animl-core.xsd         version 1.26
        * animl-technique.xsd    version 1.21
        * uv-vis.atdd            version 1.2

        Feb 8, 2007 Stuart J. Chalk
 -->
- <AnIML xmlns="urn:org:astm:animl:schema:core:draft:0.2"
   xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
   xsi:schemaLocation="urn:org:astm:animl:schema:core:draft:0.2
   http://animl.cvs.sourceforge.net/*checkout*/animl/schema/animl-core.xsd?revision=1.26"
   version="0.2">
 - <!--
  SampleSet is defined in animl-core.xsd
  -->
- <SampleSet>
- <Sample sampleID="sample0001" id="ID000001">
 - <!--
  This sample is a "Test Sample" SampleRole defined in the uv-vis.atdd
  -->
- <ParameterCategorySet>
- <ParameterCategory name="Description">
- <ParameterSet>
- <Parameter name="Name">
 - <!--
  REQUIRED
  -->
 <String>Pond spike 1.5 ppm phos</String>
  </Parameter>
- <Parameter name="Descriptive Name">
 - <!--
  OPTIONAL
  -->
 <String>Pond water spiked with 1.5 ppm arsenate</String>
  </Parameter>
- <Parameter name="Mass">
 - <!--
  OPTIONAL
  -->
 <Float32>99.983</Float32>
- <Unit label="g">
 <SIUnit exponent="1" factor="1E-03" offset="0">kg</SIUnit>
  </Unit>
  </Parameter>
- <Parameter name="Volume">
 - <!--
  OPTIONAL
  -->
 <Float32>100.0</Float32>
- <Unit label="mL">
 <SIUnit exponent="3" factor="0.000001">m</SIUnit>
```

```
    </Unit>
    </Parameter>
- <Parameter name="Concentration">
  - <!--
    OPTIONAL
    -->
  <Float32>1.5</Float32>
- <Unit label="µg/mL">
  - <!--
    ppm
    -->
  <SIUnit exponent="1" factor="0.000000001" offset="0">kg</SIUnit>
  <SIUnit exponent="-3" factor="0.000001" offset="0">kg</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="State">
  - <!--
    OPTIONAL
    -->
  - <!--
    One from solid | amorphous solid | crystalline solid | liquid | liquid crystal | gas |
     supercritical fluid | colloid | plasma | crystal
    -->
  <String>liquid</String>
    </Parameter>
- <Parameter name="Disposal Procedure">
  - <!--
    OPTIONAL
    -->
  <String>Add to heavy metal hazardous waste bottle and label</String>
    </Parameter>
- <Parameter name="Handling Precautions">
  - <!--
    OPTIONAL
    -->
  <String>Latex gloves should be used during preparation, handling, and disposal</String>
    </Parameter>
- <Parameter name="Storage Information">
  - <!--
    OPTIONAL
    -->
  <String>HDPE or LDPE bottle. Bottle color is not important.</String>
    </Parameter>
- <Parameter name="Storage Location">
  - <!--
    OPTIONAL
    -->
  <String>Shelves in the middle of the research laboratory building 10/3512</String>
    </Parameter>
- <Parameter name="Receipt Time Stamp">
  - <!--
    OPTIONAL
    -->
  <DateTime>2006-11-30T09:17:14-05:00</DateTime>
    </Parameter>
- <Parameter name="Preparation Procedure">
  - <!--
    OPTIONAL
```

```
    -->
  <String>Add 10 mL, 10 mL of filter pond water, 375 µL of 100 ppm arsenate, 0.5 mL of
    vanadomolybdate reagent, make to volume with Milli-Q water.</String>
    </Parameter>
- <Parameter name="Pressure">
  - <!--
    OPTIONAL
    -->
  <Float32>101325</Float32>
- <Unit label="Pa">
  <SIUnit exponent="-1">m</SIUnit>
  <SIUnit exponent="1">kg</SIUnit>
  <SIUnit exponent="-2">s</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Temperature">
  - <!--
    OPTIONAL
    -->
  <Float32>22.3</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Density">
  - <!--
    OPTIONAL
    -->
  <Float32>0.99983</Float32>
- <Unit label="g/mL">
  <SIUnit exponent="1" factor="0.001">kg</SIUnit>
  <SIUnit exponent="-3" factor="0.01">m</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Lot or Batch Name/Number">
  - <!--
    OPTIONAL
    -->
  <String>Arsenate spike solution</String>
    </Parameter>
- <Parameter name="Origin/Supplier">
  - <!--
    OPTIONAL
    -->
  <String>Stuart J. Chalk, University of North Florida</String>
    </Parameter>
    </ParameterSet>
- <ParameterCategorySet>
- <ParameterCategory name="Boiling point">
  - <!--
    OPTIONAL
    -->
- <ParameterSet>
- <Parameter name="Minimum Temperature">
  <Float32>99.9</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
```

```
    </Unit>
    </Parameter>
- <Parameter name="Maximum Temperature">
  <Float32>100.1</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Pressure">
  <Float32>101325</Float32>
- <Unit label="Pa">
  <SIUnit exponent="-1">m</SIUnit>
  <SIUnit exponent="1">kg</SIUnit>
  <SIUnit exponent="-2">s</SIUnit>
    </Unit>
    </Parameter>
    </ParameterSet>
    </ParameterCategory>
- <ParameterCategory name="Melting point">
  - <!--
    OPTIONAL
    -->
- <ParameterSet>
- <Parameter name="Minimum Temperature">
  <Float32>-0.1</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Maximum Temperature">
  <Float32>0.1</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Pressure">
  <Float32>101325</Float32>
- <Unit label="Pa">
  <SIUnit exponent="-1">m</SIUnit>
  <SIUnit exponent="1">kg</SIUnit>
  <SIUnit exponent="-2">s</SIUnit>
    </Unit>
    </Parameter>
    </ParameterSet>
    </ParameterCategory>
- <ParameterCategory name="Refractive Index">
- <ParameterSet>
- <Parameter name="Refractive Index">
  <Float32>1.34451</Float32>
- <Unit label="1">
  <SIUnit exponent="1" factor="1" offset="0">1</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Temperature">
  <Float32>25</Float32>
- <Unit label="°C">
```

```
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Wavelength">
  <Float32>400</Float32>
- <Unit label="nm">
  <SIUnit factor="0.000000001" exponent="1" offset="0">m</SIUnit>
    </Unit>
    </Parameter>
    </ParameterSet>
    </ParameterCategory>
    </ParameterCategorySet>
    </ParameterCategory>
- <ParameterCategory name="Substance Description">
- <ParameterSet>
- <Parameter name="Name">
  <String>Arsenate ion</String>
    </Parameter>
- <Parameter name="Descriptive Name">
  <String>Arsenate ion from sodium hydrogen arsenate</String>
    </Parameter>
- <Parameter name="Concentration">
  - <!--
    OPTIONAL
    -->
  <Float32>1.5</Float32>
- <Unit label="µg/mL">
  - <!--
    ppm
    -->
  <SIUnit exponent="1" factor="0.000000001" offset="0">kg</SIUnit>
  <SIUnit exponent="-3" factor="0.000001" offset="0">kg</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Molecular Formula">
  <String>AsO4</String>
    </Parameter>
- <Parameter name="Molecular Mass">
  <Float32>138.92</Float32>
- <Unit label="g/mol">
  <SIUnit exponent="1" factor="0.001" offset="0">kg</SIUnit>
  <SIUnit exponent="-1" factor="1" offset="0">mol</SIUnit>
    </Unit>
    </Parameter>
    </ParameterSet>
- <ParameterCategorySet>
- <ParameterCategory name="Chemical Structure">
- <ParameterSet>
- <Parameter name="SMILES">
  <String>O=[As](O)(O)[O-]</String>
    </Parameter>
- <Parameter name="Wiswesser">
  <String>Not available</String>
    </Parameter>
- <Parameter name="MOL File">
  - <String>
```

```
- <![CDATA[
                                        Marvin  08050516092D

  5  4  0  0  0  0            999 V2000
    1.4289    0.1650    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    0.7145   -0.2475    0.0000 As  0  0  0  0  0  0  0  0  0  0  0  0
    0.0000    0.1650    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7145   -0.2475    0.0000 As  0  0  0  0  0  0  0  0  0  0  0  0
   -1.4289    0.1650    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  2  3  1  0  0  0  0
  3  4  1  0  0  0  0
  4  5  2  0  0  0  0
M  END

]]>
</String>
</Parameter>
- <Parameter name="CML">
  - <EmbeddedXML>
    - <![CDATA[
    <?xml version="1.0" ?>
    <molecule id=\"ARSENATE\" title=\"arsenate\" dictRef=\"dictARSENATE\">
       <atomArray>
        <atom id=\"ARSENATE-atom1\" elementType=\"AS\" x2=\"0.0\" y2=\"0.0\"/>
        <atom id=\"ARSENATE-atom2\" elementType=\"O\" x2=\"0.9961977\" y2=\"0.0\"
    formalCharge=\"-1\"/>
        <atom id=\"ARSENATE-atom3\" elementType=\"O\" x2=\"0.0\" y2=\"0.9961977\"
    formalCharge=\"-1\"/>
        <atom id=\"ARSENATE-atom4\" elementType=\"O\" x2=\"0.0\" y2=\"-1.0\" formalCharge=\"-
    1\"/>
        <atom id=\"ARSENATE-atom5\" elementType=\"O\" x2=\"-1.0\" y2=\"0.0\"/>
       </atomArray>
       <bondArray>
        <bond id=\"ARSENATE-bond1\" atomRefs=\"ARSENATE-atom5 ARSENATE-atom1\" order=\"2\"/>
        <bond id=\"ARSENATE-bond2\" atomRefs=\"ARSENATE-atom4 ARSENATE-atom1\" order=\"1\"/>
        <bond id=\"ARSENATE-bond3\" atomRefs=\"ARSENATE-atom3 ARSENATE-atom1\" order=\"1\"/>
        <bond id=\"ARSENATE-bond4\" atomRefs=\"ARSENATE-atom2 ARSENATE-atom1\" order=\"1\"/>
       </bondArray>
       <formula concise=\"O 4 AS 1\" formalCharge=\"-3\"/>
       <float title=\"molecularWeight\" units=\"g/mol\">138.919</float>
       <string title=\"smiles\">[As]([O-1])([O-1])(=O)[O-1]</string>
      </molecule>

    ]]>
    </EmbeddedXML>
    </Parameter>
    </ParameterSet>
    </ParameterCategory>
- <ParameterCategory name="Chemical Identifier">
- <ParameterSet>
- <Parameter name="CAS Name">
  <String>Arsenate ion</String>
    </Parameter>
- <Parameter name="CAS Registry Number">
  <String>15584-04-0</String>
    </Parameter>
- <Parameter name="Beilstein Lawson Number">
  <String>Not available</String>
    </Parameter>
- <Parameter name="InChI">
```

```
<String>InChI=1/AsH3O4.Na/c2-1(3,4)5;/h(H3,2,3,4,5);/q;+1/p-1</String>
  </Parameter>
- <Parameter name="CML">
  - <EmbeddedXML>
      - <![CDATA[
      <?xml version="1.0" ?>
      <molecule id=\"ARSENATE\" title=\"arsenate\" dictRef=\"dictARSENATE\">
         <atomArray>
          <atom id=\"ARSENATE-atom1\" elementType=\"AS\" x2=\"0.0\" y2=\"0.0\"/>
          <atom id=\"ARSENATE-atom2\" elementType=\"O\" x2=\"0.9961977\" y2=\"0.0\"
      formalCharge=\"-1\"/>
          <atom id=\"ARSENATE-atom3\" elementType=\"O\" x2=\"0.0\" y2=\"0.9961977\"
      formalCharge=\"-1\"/>
          <atom id=\"ARSENATE-atom4\" elementType=\"O\" x2=\"0.0\" y2=\"-1.0\" formalCharge=\"-
      1\"/>
          <atom id=\"ARSENATE-atom5\" elementType=\"O\" x2=\"-1.0\" y2=\"0.0\"/>
         </atomArray>
         <bondArray>
          <bond id=\"ARSENATE-bond1\" atomRefs=\"ARSENATE-atom5 ARSENATE-atom1\" order=\"2\"/>
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<Float64>0.0507</Float64>
    </IndividualValueSet>
- <Unit label="Absorbance">
  <SIUnit exponent="1" factor="1" offset="0">1</SIUnit>
    </Unit>
    </Vector>
    </VectorSet>
- <ParameterCategorySet>
- <ParameterCategory name="Measurement Description">
  - <!--
    REQUIRED
    -->
```

```
- <ParameterSet>
- <Parameter name="Identifier">
  - <!--
    REQUIRED
     -->
  <String>Pond spike 1.5 ppm phos spectrum</String>
    </Parameter>
- <Parameter name="Title">
  - <!--
    OPTIONAL
     -->
  <String>UV/Vis Spectrum of Pondwater Spiked with 1.5 ppm Arsenate</String>
    </Parameter>
- <Parameter name="Project">
  - <!--
    OPTIONAL
     -->
  <String>Arsenate research</String>
    </Parameter>
- <Parameter name="Method Reference">
  - <!--
    OPTIONAL
     -->
  <String>Research Notebook Chalk7, Page 32</String>
    </Parameter>
- <Parameter name="Scan Number">
  - <!--
    OPTIONAL
     -->
  <INT>1</INT>
    </Parameter>
- <Parameter name="Scan Duration">
  - <!--
    OPTIONAL
     -->
  <Float32>100.0</Float32>
- <Unit label="s">
  <SIUnit exponent="1" factor="1" offset="0">s</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Experiment Duration">
  - <!--
    REQUIRED
     -->
  <Float32>100.0</Float32>
- <Unit label="s">
  <SIUnit exponent="1" factor="1" offset="0">s</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Sample Path Length">
  - <!--
    REQUIRED
     -->
  <Float32>1.0</Float32>
- <Unit label="cm">
  <SIUnit exponent="1" factor="0.01">m</SIUnit>
    </Unit>
```

```
    </Parameter>
    </ParameterSet>
- <ParameterCategorySet>
- <ParameterCategory name="Temperature Range">
  - <!--
    OPTIONAL
    -->
- <ParameterSet>
- <Parameter name="Min">
  - <!--
    REQUIRED
    -->
  <Float32>22.0</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Max">
  - <!--
    OPTIONAL
    -->
  <Float32>23.0</Float32>
- <Unit label="°C">
  <SIUnit offset="-273.15">K</SIUnit>
    </Unit>
    </Parameter>
    </ParameterSet>
    </ParameterCategory>
    </ParameterCategorySet>
    </ParameterCategory>
- <ParameterCategory name="Instrument Properties">
  - <!--
    REQUIRED
    -->
- <ParameterSet>
- <Parameter name="Resolution">
  - <!--
    REQUIRED
    -->
  <Float32>1.0</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Scan Mode">
  - <!--
    REQUIRED
    -->
  <String>Spectrum</String>
    </Parameter>
- <Parameter name="Spectral Slit Width">
  - <!--
    OPTIONAL
    -->
  <Float32>2.0</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
```

```
    </Unit>
    </Parameter>
- <Parameter name="Integration Time">
  - <!--
    OPTIONAL
    -->
  <Float32>0.5</Float32>
- <Unit label="s">
  <SIUnit exponent="1" factor="1" offset="0">s</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Spectrum Derivatization Method">
  - <!--
    REQUIRED
    -->
  <INT>0</INT>
    </Parameter>
- <Parameter name="Derivatization Algorithm Description">
  - <!--
    OPTIONAL
    -->
  <String>None</String>
    </Parameter>
- <Parameter name="Background Correction Type">
  - <!--
    OPTIONAL
    -->
  <String>Dual beam measurement against reagent blank</String>
    </Parameter>
- <Parameter name="Straylight Correction">
  - <!--
    OPTIONAL
    -->
  <Boolean>true</Boolean>
    </Parameter>
- <Parameter name="Signal to Noise Ratio">
  - <!--
    OPTIONAL
    -->
  <Float32>250.1</Float32>
- <Unit label="S/N">
  <SIUnit exponent="1" factor="1" offset="0">1</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Filter">
  - <!--
    OPTIONAL
    -->
  <String>None</String>
    </Parameter>
- <Parameter name="Slit Width">
  - <!--
    REQUIRED
    -->
  <Float32>2.0</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
```

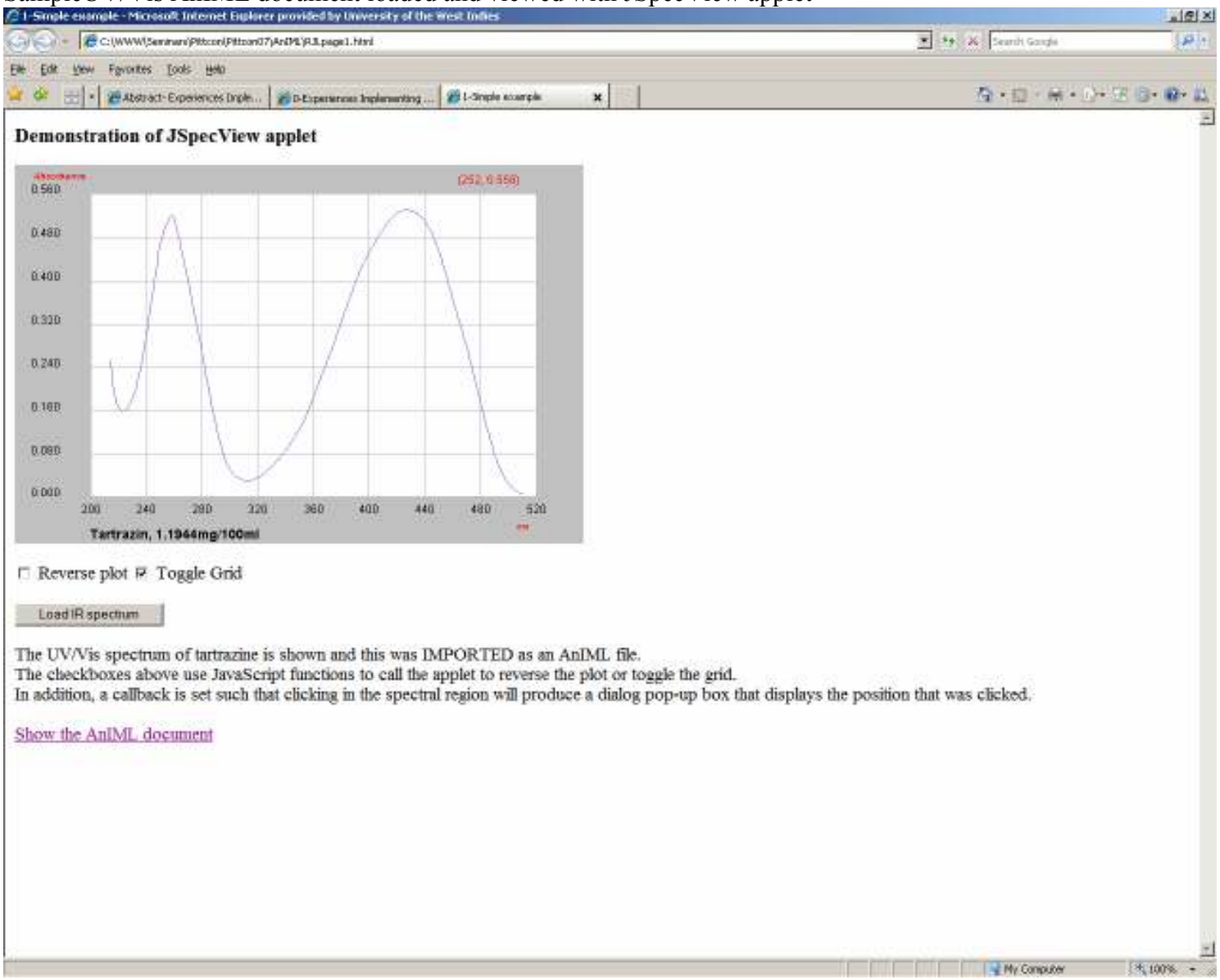
```
    </Unit>
    </Parameter>
- <Parameter name="Detector Types">
  - <!--
    OPTIONAL
    -->
  <String>Hamamatsu PMT internal to UniCam UV-4</String>
    </Parameter>
- <Parameter name="Scan Speed">
  - <!--
    OPTIONAL
    -->
  <Float32>2.0</Float32>
- <Unit label="nm/s">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
  <SIUnit exponent="-1" factor="1" offset="0">s</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Point Separation">
  - <!--
    OPTIONAL
    -->
  <Float32>1.0</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Sample Holder">
  - <!--
    OPTIONAL
    -->
  <String>Hellma UV transparent 1.0 cm cuvette</String>
    </Parameter>
- <Parameter name="Sample Position">
  - <!--
    OPTIONAL
    -->
  <INT>1</INT>
    </Parameter>
    </ParameterSet>
- <ParameterCategorySet>
- <ParameterCategory name="Spectral Bandwidth Range">
  - <!--
    OPTIONAL
    -->
- <ParameterSet>
- <Parameter name="Min">
  - <!--
    REQUIRED
    -->
  <Float32>-0.25</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Max">
  - <!--
```

```
    OPTIONAL
     -->
  <Float32>+0.25</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
     </Unit>
     </Parameter>
     </ParameterSet>
     </ParameterCategory>
- <ParameterCategory name="Wavelength Range">
  - <!--
    REQUIRED
     -->
- <ParameterSet>
- <Parameter name="Min">
  - <!--
    REQUIRED
     -->
  <Float32>200</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
     </Unit>
     </Parameter>
- <Parameter name="Max">
  - <!--
    REQUIRED
     -->
  <Float32>400</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
     </Unit>
     </Parameter>
     </ParameterSet>
     </ParameterCategory>
- <ParameterCategory name="Absorbance Range">
  - <!--
    OPTIONAL
     -->
- <ParameterSet>
- <Parameter name="Min">
  - <!--
    REQUIRED
     -->
  <Float32>-0.1</Float32>
- <Unit label="A">
  <SIUnit exponent="1" factor="1" offset="0">1</SIUnit>
     </Unit>
     </Parameter>
- <Parameter name="Max">
  - <!--
    REQUIRED
     -->
  <Float32>6.000</Float32>
- <Unit label="A">
  <SIUnit exponent="1" factor="1" offset="0">1</SIUnit>
     </Unit>
     </Parameter>
```

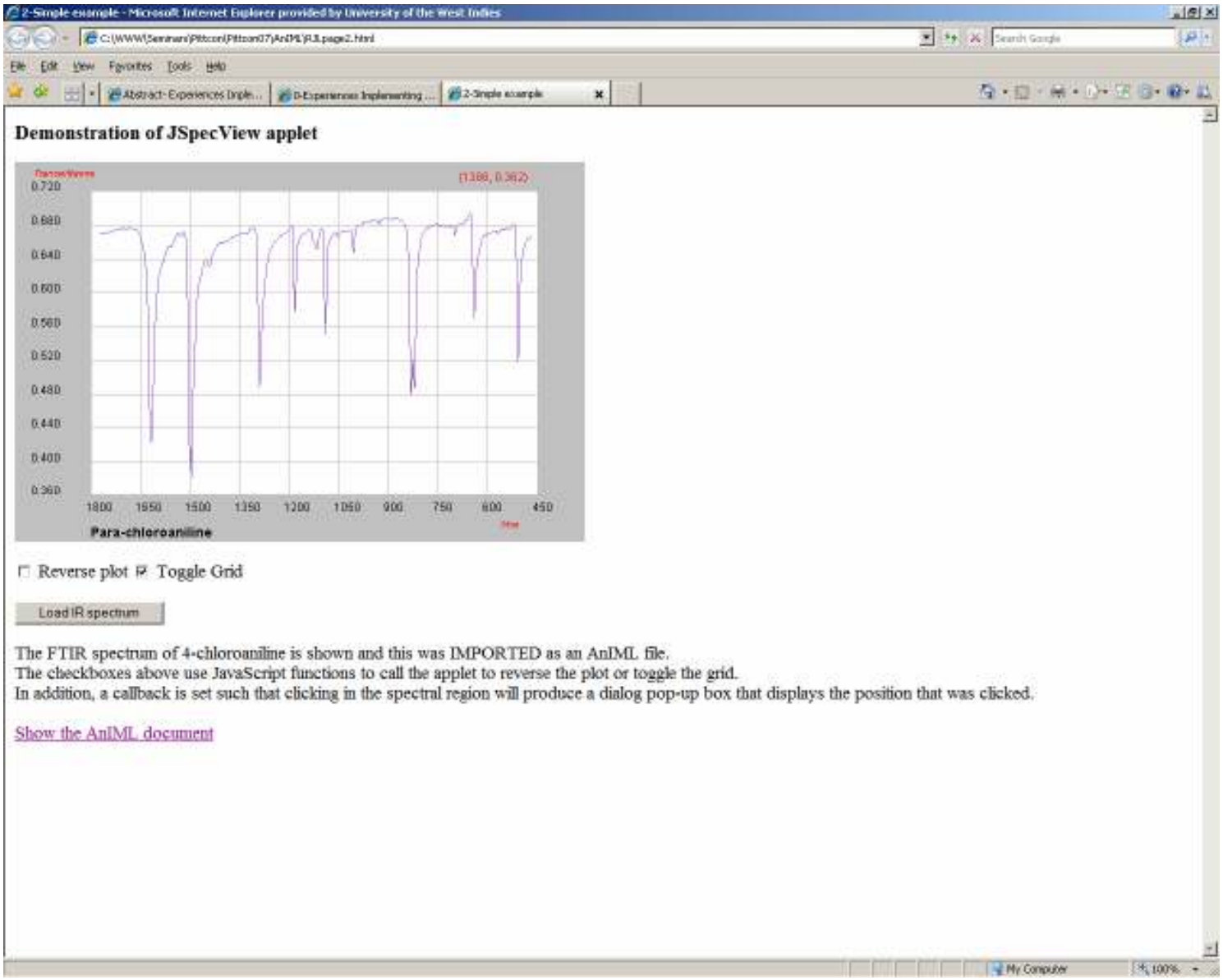
```
    </ParameterSet>
    </ParameterCategory>
- <ParameterCategory name="Source Used">
  - <!--
    OPTIONAL
    -->
- <ParameterSet>
- <Parameter name="Source Type">
  - <!--
    REQUIRED
    -->
  <String>Deuterium Lamp</String>
    </Parameter>
- <Parameter name="Min">
  - <!--
    REQUIRED
    -->
  <Float32>190.0</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
    </Unit>
    </Parameter>
- <Parameter name="Max">
  - <!--
    REQUIRED
    -->
  <Float32>400.0</Float32>
- <Unit label="nm">
  <SIUnit exponent="1" factor="0.000000001" offset="0">m</SIUnit>
    </Unit>
    </Parameter>
    </ParameterSet>
    </ParameterCategory>
    </ParameterCategorySet>
    </ParameterCategory>
    </ParameterCategorySet>
    </Page>
    </PageSet>
- <TrackingTagSet>
  <TrackingTag name="Research area" value="Arsenate chemistry" />
    </TrackingTagSet>
    </ExperimentStep>
    </ExperimentStepSet>
  - <!--
    AuditTrial is defined in animl-core.xsd
    -->
- <AuditTrail>
- <LogEntry>
  <Timestamp>2006-11-30T09:17:14-05:00</Timestamp>
- <UserInformation userType="human">
  <Name>Stuart Chalk</Name>
  <Email>schalk@unf.edu</Email>
  <Phone>0101-904-620-1938</Phone>
  <Location>Department of Chemistry and Physics, University of North Florida, 4567 St Johns Bluff Rd
    S, Jacksonville, FL 32224 USA</Location>
    </UserInformation>
  <Action>created</Action>
```

```
<Reason>As a working example of AnIML</Reason>
<Description>An example XML data file that shows all the elements, attributes, and structure of the
   animl specficiation as defined by the versions indicated at the top of this XML file</Description>
<Reference>ID000001</Reference>
- <!--
 There can be multiple references here
  -->
  </LogEntry>
  </AuditTrail>
- <!--
 SignatureSet is defined in xmldsig-core-schema.xsd via animl-core.xsd
  -->
- <SignatureSet>
- <Signature>
- <SignedInfo xmlns="http://www.w3.org/2000/09/xmldsig#">
<CanonicalizationMethod Algorithm="" />
<SignatureMethod Algorithm="" />
- <Reference>
<DigestMethod Algorithm="" />
<DigestValue />
  </Reference>
  </SignedInfo>
<SignatureValue xmlns="http://www.w3.org/2000/09/xmldsig#" />
  </Signature>
  </SignatureSet>
  </AnIML>
```

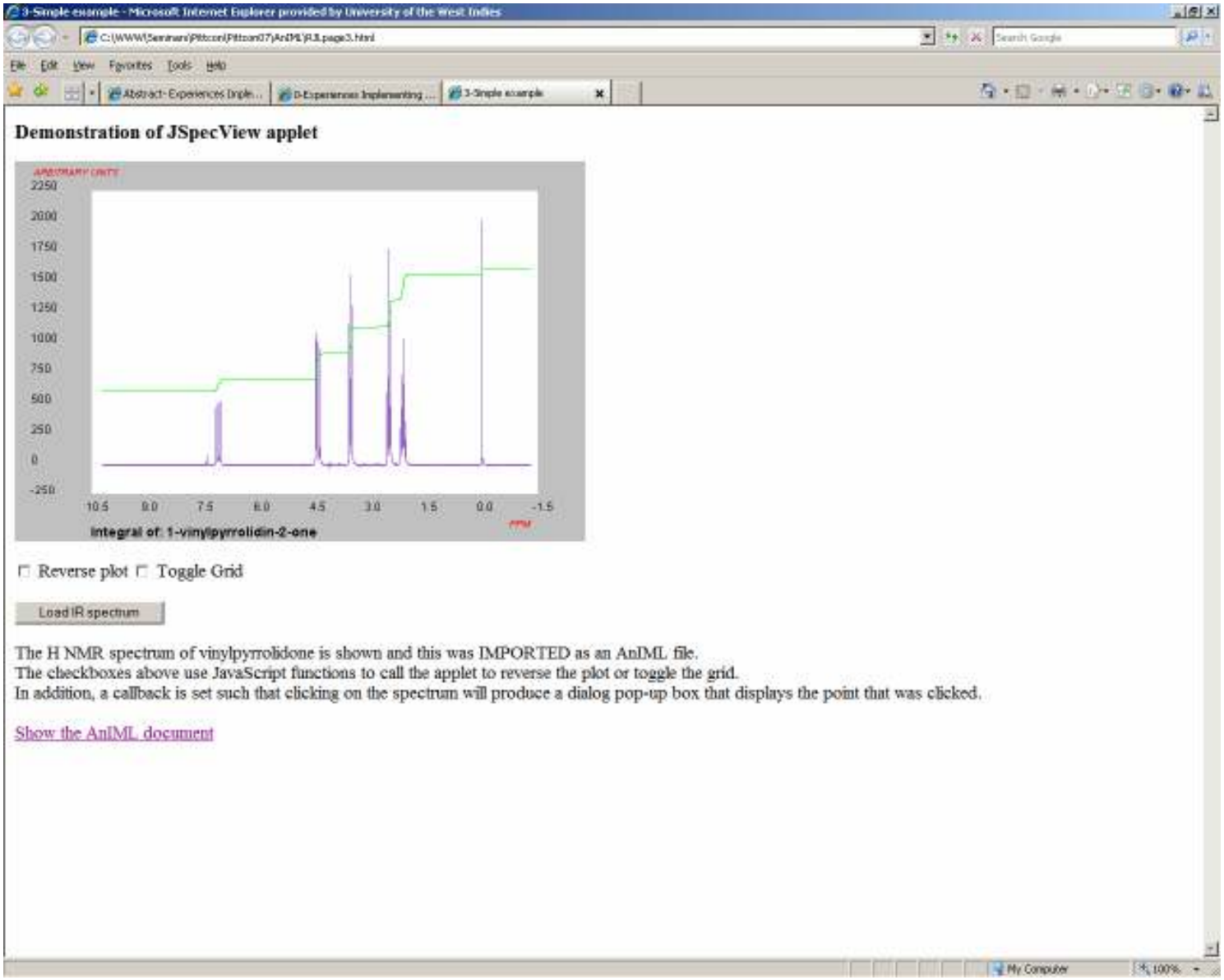
SampleUV/Vis AnIML document loaded and viewed with JSpecView applet



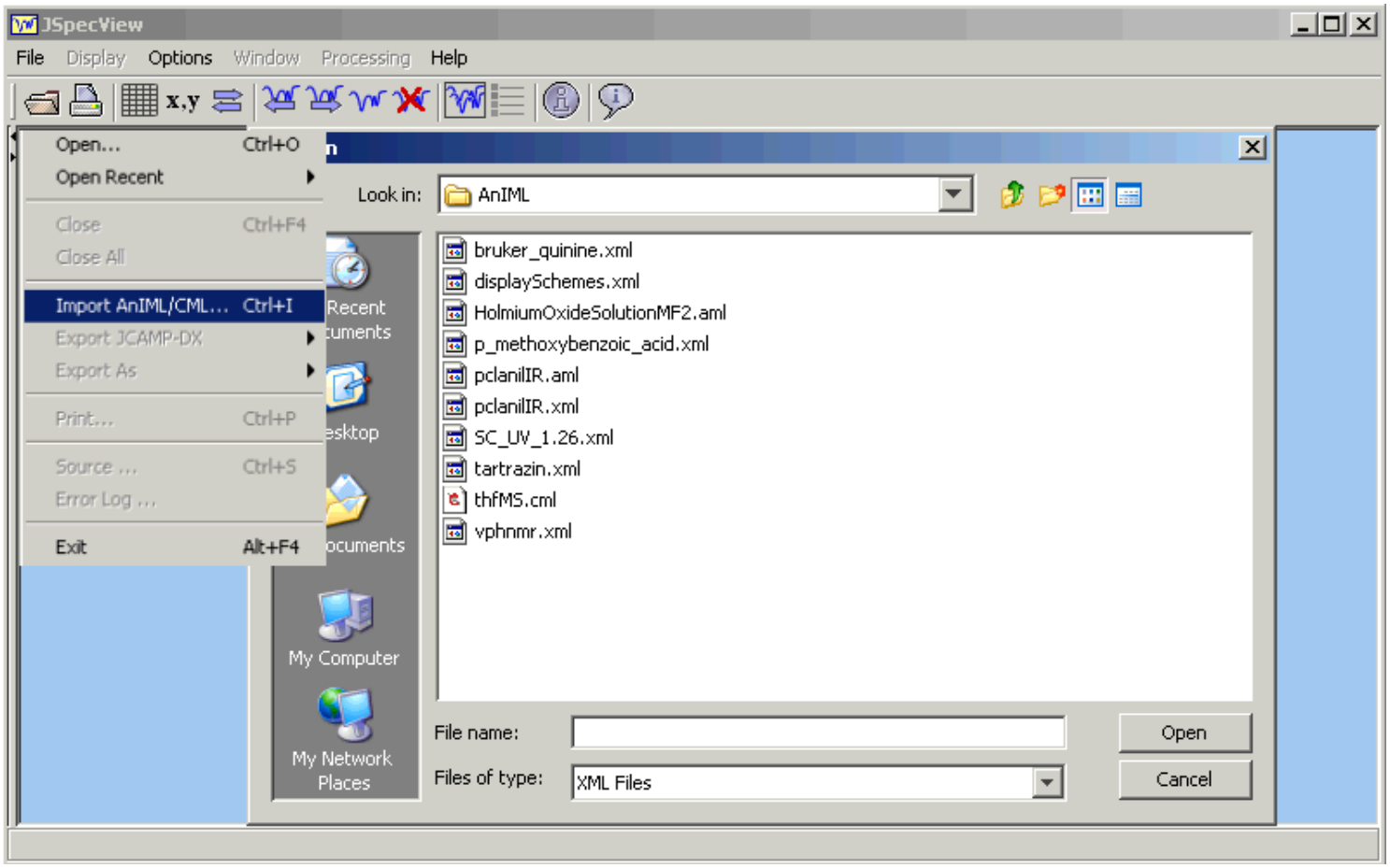
Sample IR AnIML document loaded and viewed with JSpecView applet

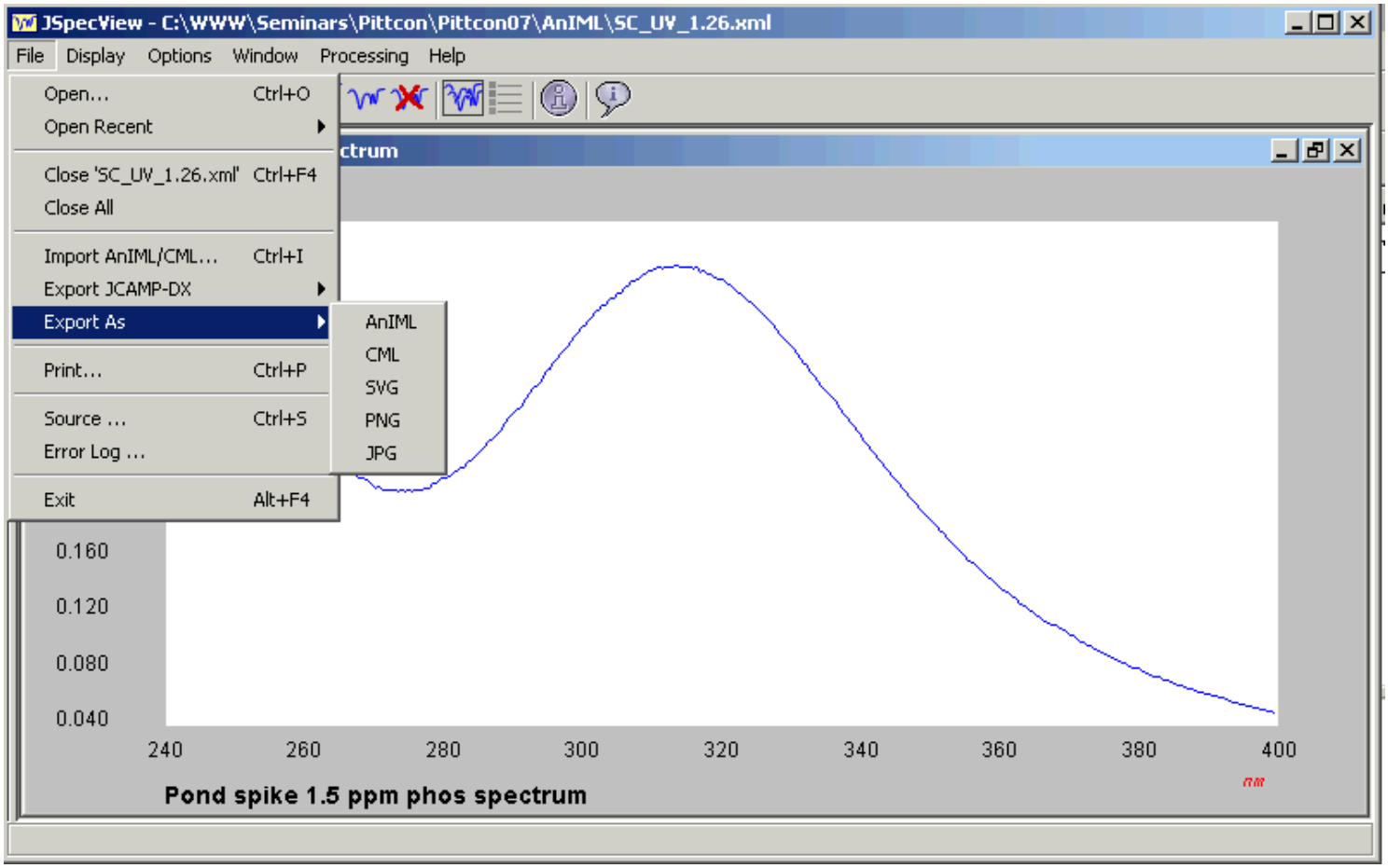


Sample NMR AnIML document loaded and viewed with JSpecView applet

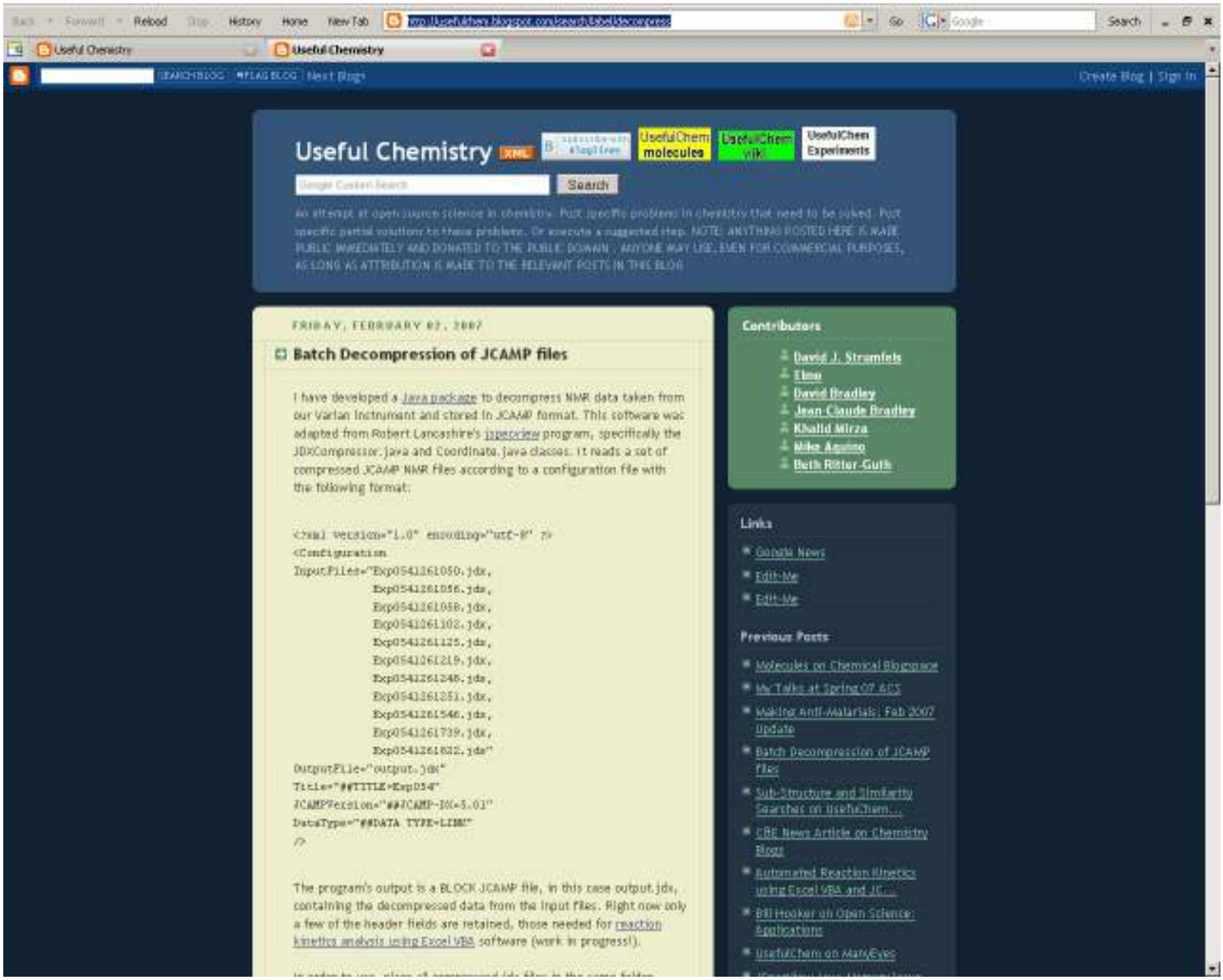


Sample UV/Vis AnIML document loaded and viewed with JSpecView application



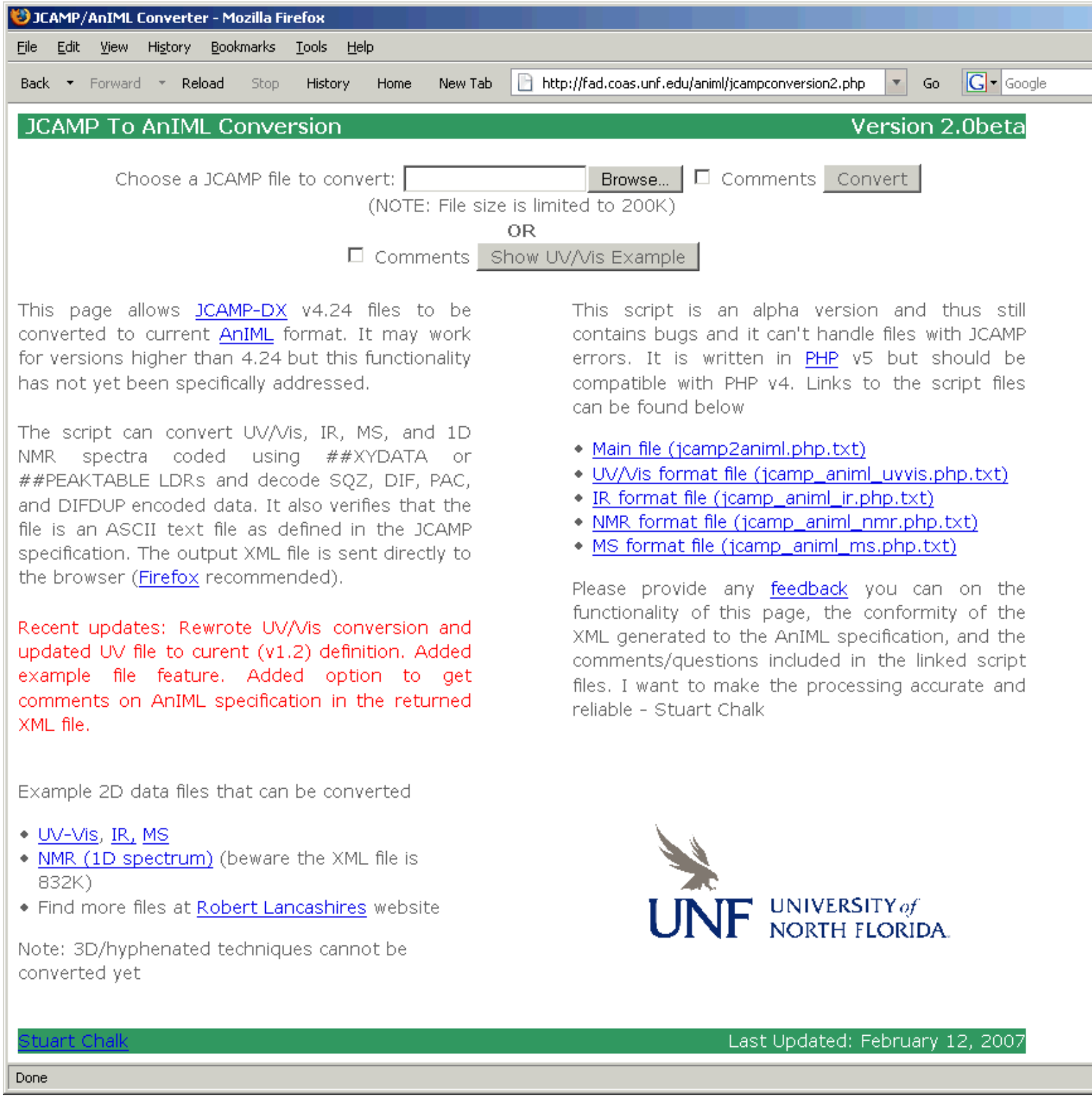


Open Source enhancements of the JSpecView code for batch conversion of JCAMP-DX files.



On-line conversion of JCAMP-DX files to AnIML

http://fad.coas.unf.edu/animl/jcampconversion2.php



The StAX method used in JSpecView is XMLEventReader**.**

According to the Sun tutorial, JavaWSTutorial.pdf found at
http://java.sun.com/webservices/docs/1.6/tutorial/doc/JavaWSTutorial.pdf
"XMLStreamReader is more efficient, but XMLEventReader is easier to use, as all the information related to a particular event is encapsulated in a returned XMLEvent object."

Creating an Input Factory

The first step is to create a new instance of XMLInputFactory:

```
    XMLInputFactory factory = XMLInputFactory.newInstance();
    System.out.println("FACTORY: " + factory);
```

Creating an Event Reader

The next step is to create an instance of XMLEventReader:

```
    XMLEventReader r = factory.createXMLEventReader(filename, new
         FileInputStream(filename));
```

Creating an Event Iterator

The third step is to create an event iterator:

```
    XMLEventReader r = factory.createXMLEventReader(filename, new
         FileInputStream(filename));
    while(r.hasNext()) {
          XMLEvent e = r.nextEvent();
          System.out.println(e.toString());
     }
```

Getting the Event Stream

The final step is to get the underlying event stream:

```
public final static String getEventTypeString(int eventType) {
       switch (eventType) {
              case XMLEvent.START_ELEMENT:
                   return "START_ELEMENT";
              case XMLEvent.END_ELEMENT:
                   return "END_ELEMENT";
              case XMLEvent.PROCESSING_INSTRUCTION:
                   return "PROCESSING_INSTRUCTION";
              case XMLEvent.CHARACTERS:
                   return "CHARACTERS";
              case XMLEvent.COMMENT:
                   return "COMMENT";
              case XMLEvent.START_DOCUMENT:
                   return "START_DOCUMENT";
              case XMLEvent.END_DOCUMENT:
```

```
                return "END_DOCUMENT";
            case XMLEvent.ENTITY_REFERENCE:
                return "ENTITY_REFERENCE";
            case XMLEvent.ATTRIBUTE:
                return "ATTRIBUTE";
            case XMLEvent.DTD:
                return "DTD";
            case XMLEvent.CDATA:
                return "CDATA";
            case XMLEvent.SPACE:
                return "SPACE";
        }
return "UNKNOWN_EVENT_TYPE " + "," + eventType;
}
```

Experiences Implementing AnIML Viewers and Converters

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- WWW feedback from http://wwwchem.uwimona.edu.jm and http://jspecview.sourceforge.net

last modified 14th February 2007.