

Overview: Accession

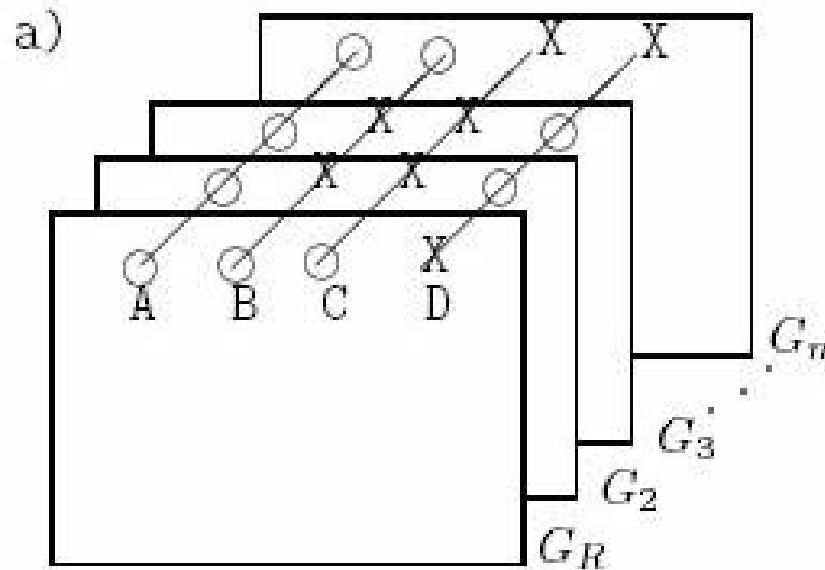
Data Accessioning Program

<http://open2dprot.sourceforge.net/Accession>

Introduction

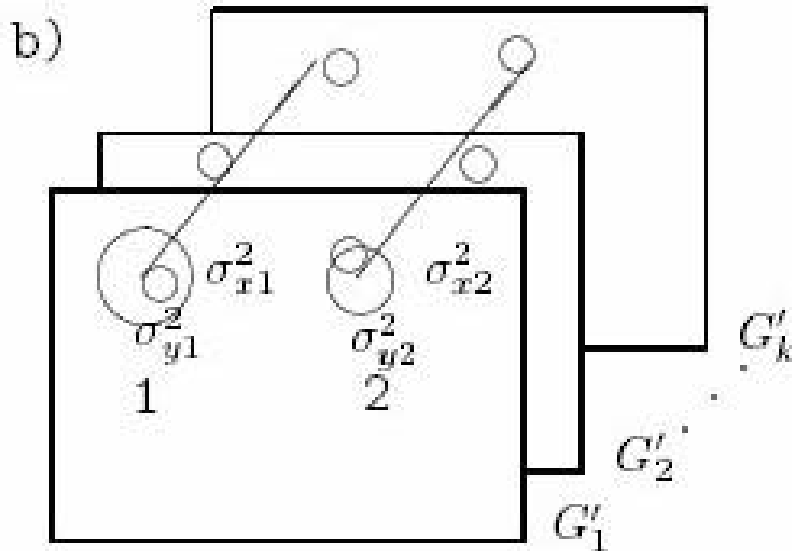
- Data must be accessioned or entered into the program database. This consists of several activities:
- 1. Entering the name of the sample and sample information
- 2. Entering the Region Of Interest of sample
- 3. Entering sample calibration info if any

Composite Samples Database (CSD) Paradigm



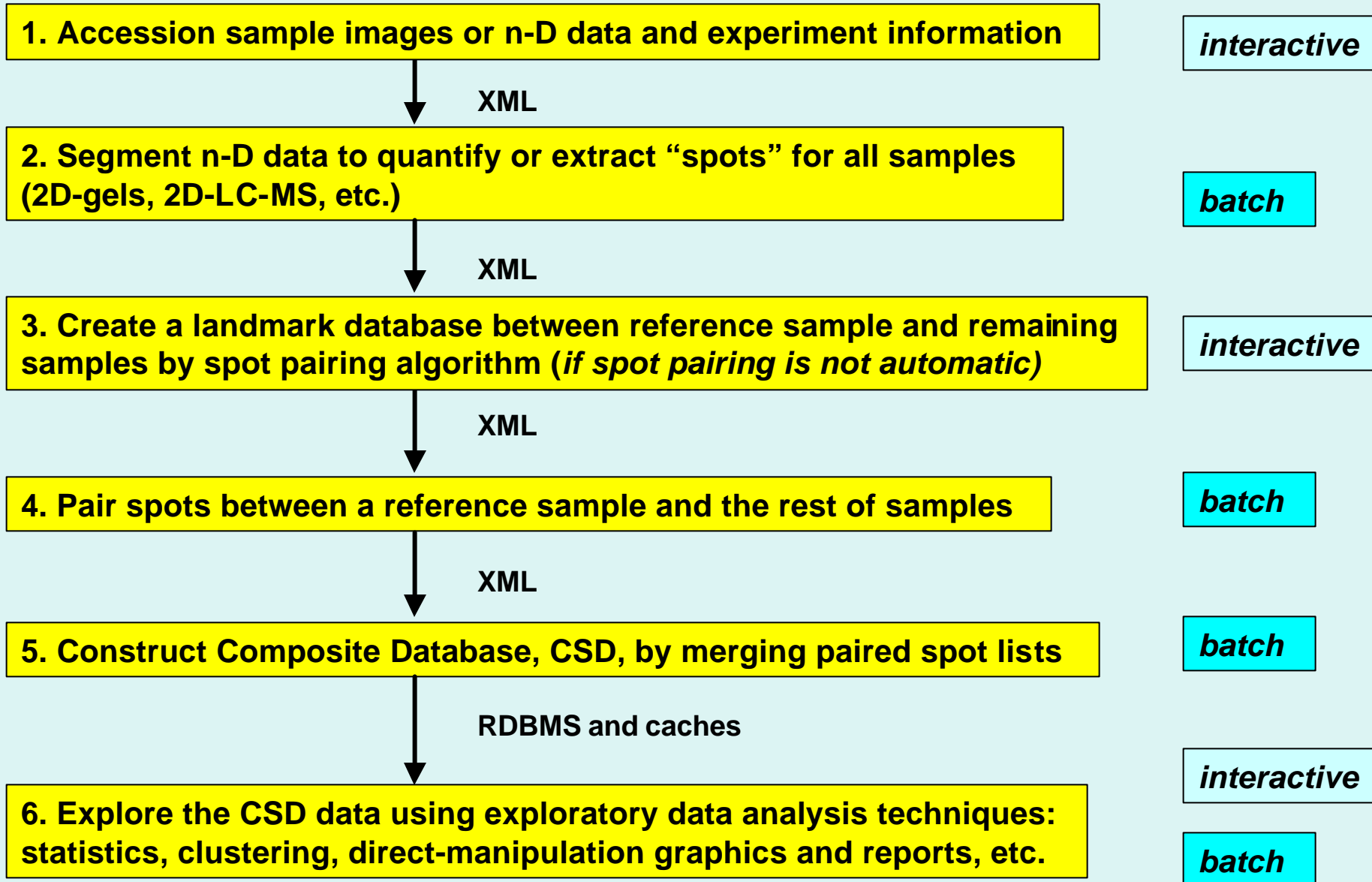
Proteomic composite samples database (CSD) consisting of a set of n samples G_1, G_2, \dots, G_n with representative sample $G_r = G_1$

Expression profiles A, B, C, ...



A canonical sample database is a statistical representation of the CSD spot geometry and quantification that could be used for data mining

Basic Open n-D Analysis Pipeline



Initial Open n-D Data-Mining Tools



- **Accession n-D sample images or n-D data and experiment data**
- **Quantify 'spots' from sample images or peptide clusters**
- **Pair spots between samples and a reference sample**
- **Construct composite sample database for exploratory data analysis**
- Manage subsets of proteins in the database
- Manage replicate samples and condition sets of samples
- Analyze expression profiles for multiple conditions
- Data-filter protein sets by statistics, clustering, set membership
- Direct-manipulation of data in graphics, spreadsheets
- Integrate R language statistical, clustering, classifiers, class prediction, and other methods
- Integrate access to Internet proteomic/genomic/function data servers for user-specified protein sets

Open2Dprot Pipeline Subprojects

Open2Dprot pipeline subprojects




[Open2Dprot](#) consists of a series of coordinated [Open2Dprot pipeline processing modules](#). By using XML as the "glue" between modules, it is possible to substitute alternate modules at the various pipeline steps. As pipeline modules and alternate modules become available, they will be added to this table. *We encourage the donation of alternate pipeline processing modules which will be added to this table.*

We will be using a common [O2Plib library](#) in the Open2Dprot pipeline modules. This will help ensure that they use the same conventions, data structures and XML data interchange formats.

| Subproject Home | Download | Documentation | Overview (PDF) | PDF documents | Version | Revision history | Status | Pipeline step |
|---|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|--------------------------|--|---------------|
| Open2Dprot | (see below) | Open2Dprot | Open2Dprot | Open2Dprot | Open2Dprot | Open2Dprot | Open2Dprot <i>design prototype</i> | - |
| Accession | Accession | Accession | Accession | Accession | Accession | Accession | Accession <i>pre-alpha</i> | [1] |
|  Seg2Dgel | Seg2Dgel | Seg2Dgel | Seg2Dgel | Seg2Dgel | Seg2Dgel | Seg2Dgel | Seg2Dgel <i>pre-alpha</i> | [2] |
| Landmark | Landmark | Landmark | Landmark | Landmark | Landmark | Landmark | Landmark <i>pre-alpha</i> | [3] |
|  CmpSpots | CmpSpots | CmpSpots | CmpSpots | CmpSpots | CmpSpots | CmpSpots | CmpSpots <i>pre-alpha</i> | [4] |
| BuildCSD | BuildCSD | BuildCSD | BuildCSD | BuildCSD | BuildCSD | BuildCSD | BuildCSD <i>design prototype</i> | [5] |
| CSDminer | CSDminer | CSDminer | CSDminer | CSDminer | CSDminer | CSDminer | CSDminer <i>design prototype</i> | [6] |
| O2Plib | O2Plib.jar | O2Plib | O2Plib | O2Plib | O2Plib | O2Plib | O2Plib <i>pre-alpha</i> | --common-- |

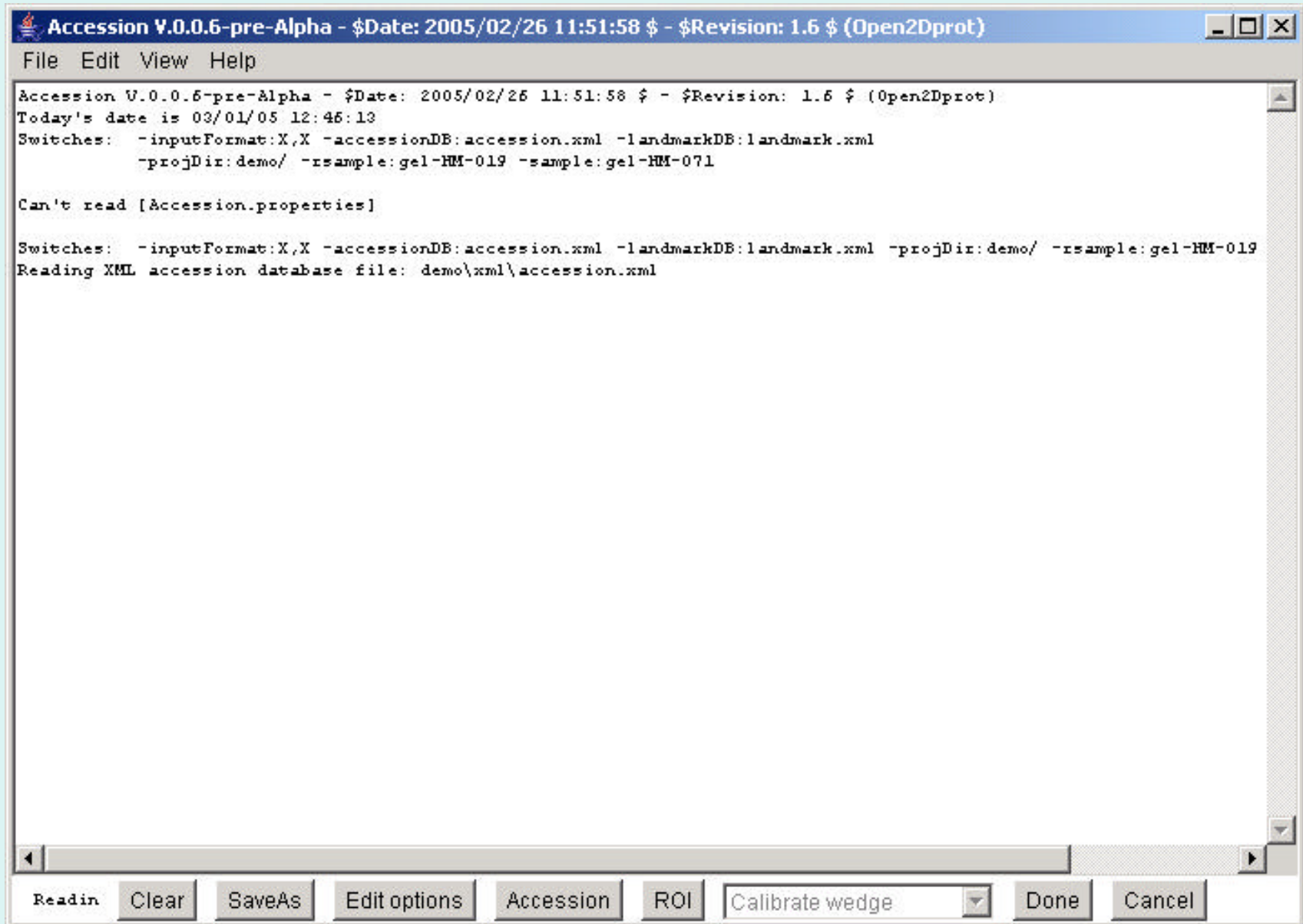
Associated or Related Projects

We had added some additional non-pipeline open source projects that may use similar data or common software modules. They may be useful for performing other types of analysis on data used by Open2Dprot or alternate types of analyses.

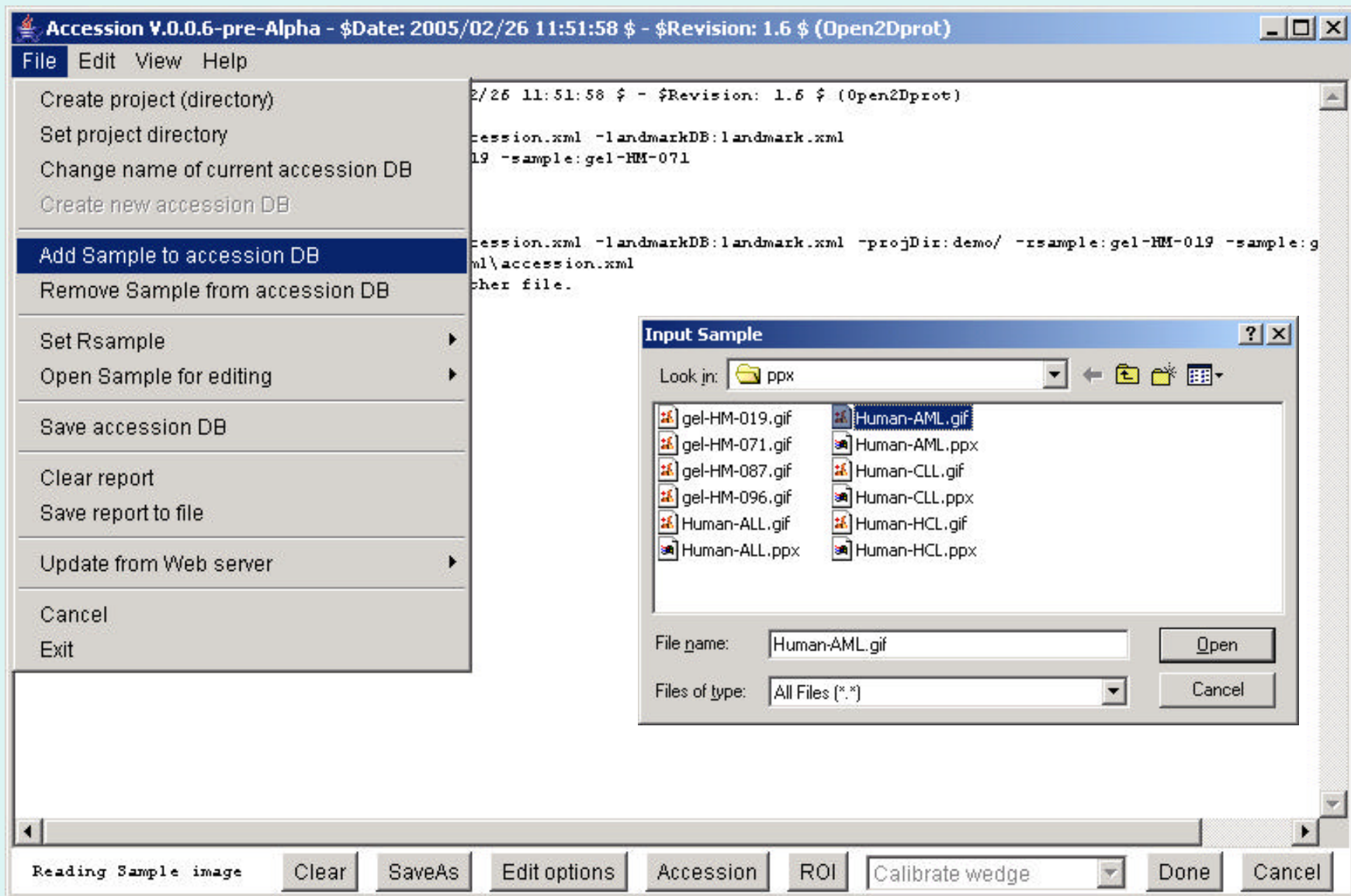
| Contributed Project Home | Download | Documentation | Overview (PDF) | PDF documents | Version | Revision history | Status |
|---|----------------------------|---------------------------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|
|  Flicker | Flicker | Flicker | Flicker | Flicker | Flicker | Flicker | Flicker |
|  MAExplorer | MAExplorer | MAExplorer | MAExplorer | MAExplorer | MAExplorer | MAExplorer | MAExplorer |
|  ProtPlot | Protplot | TMAP (ProtPlot) | ProtPlot | ProtPlot | ProtPlot | ProtPlot | --- |
| xxx | xxx | xxx | xxx | xxx | xxx | xxx | xxx |

09-12-2004

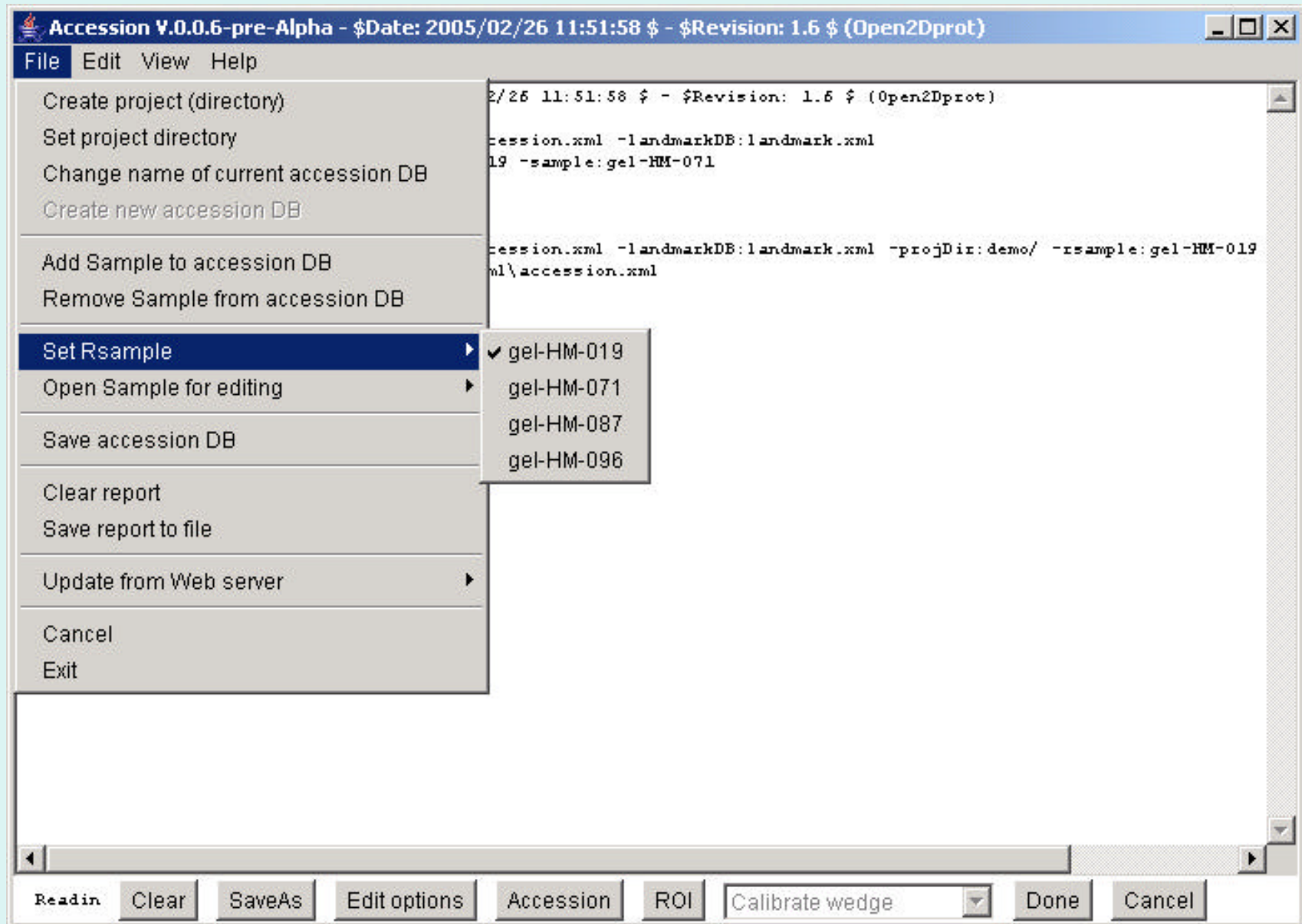
Main Window



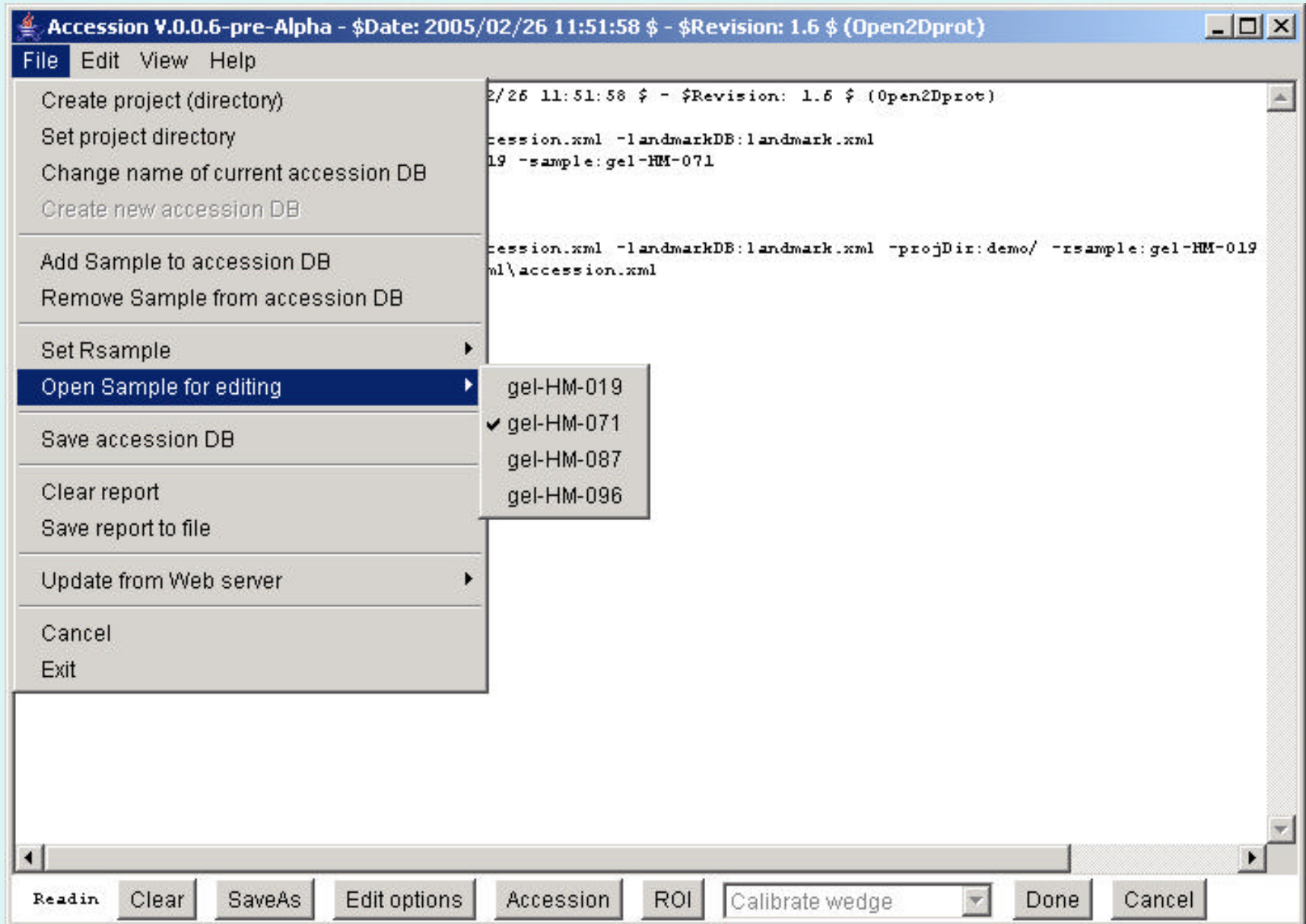
File Menu – Add New Sample



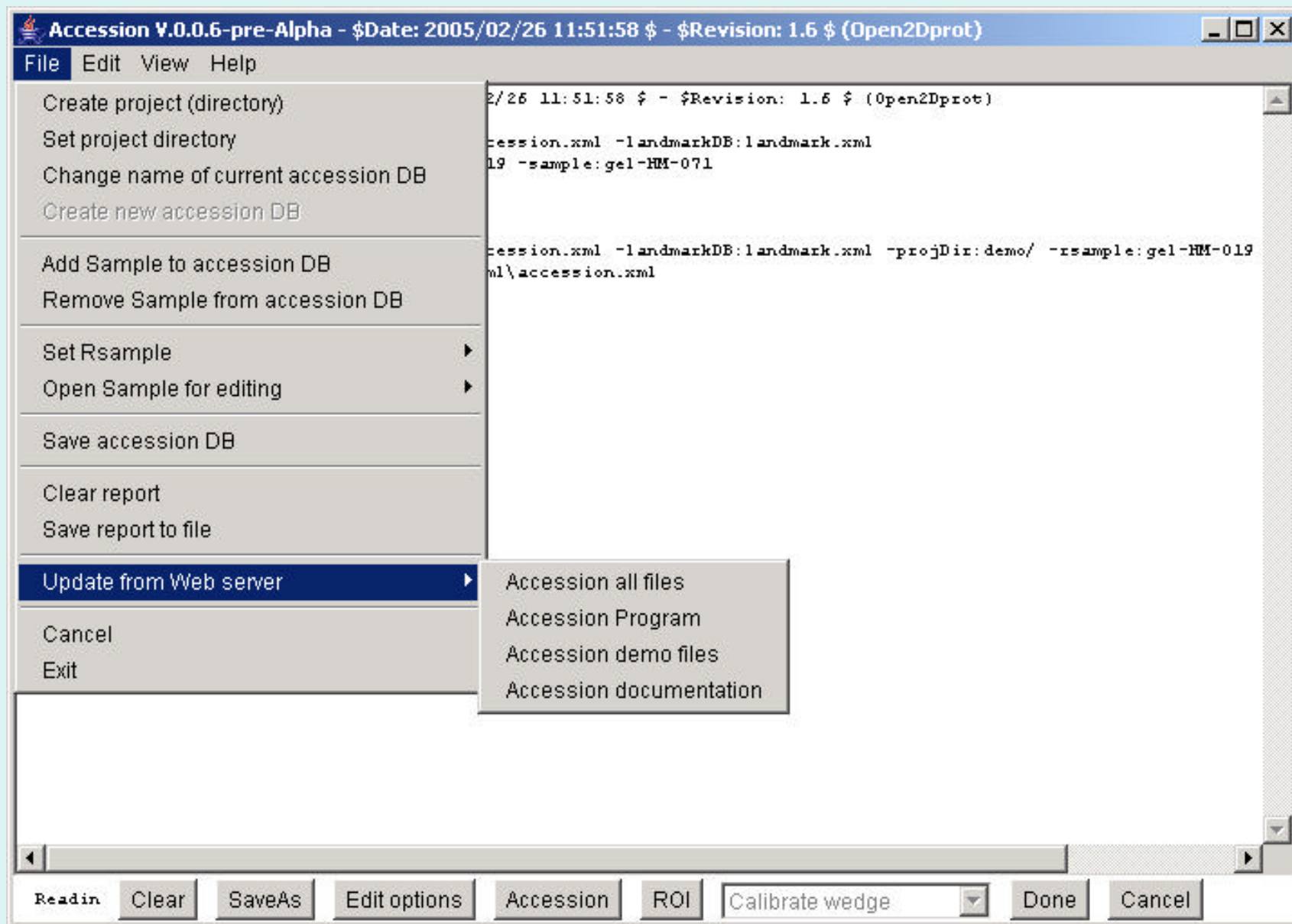
File Menu - Select Reference Sample



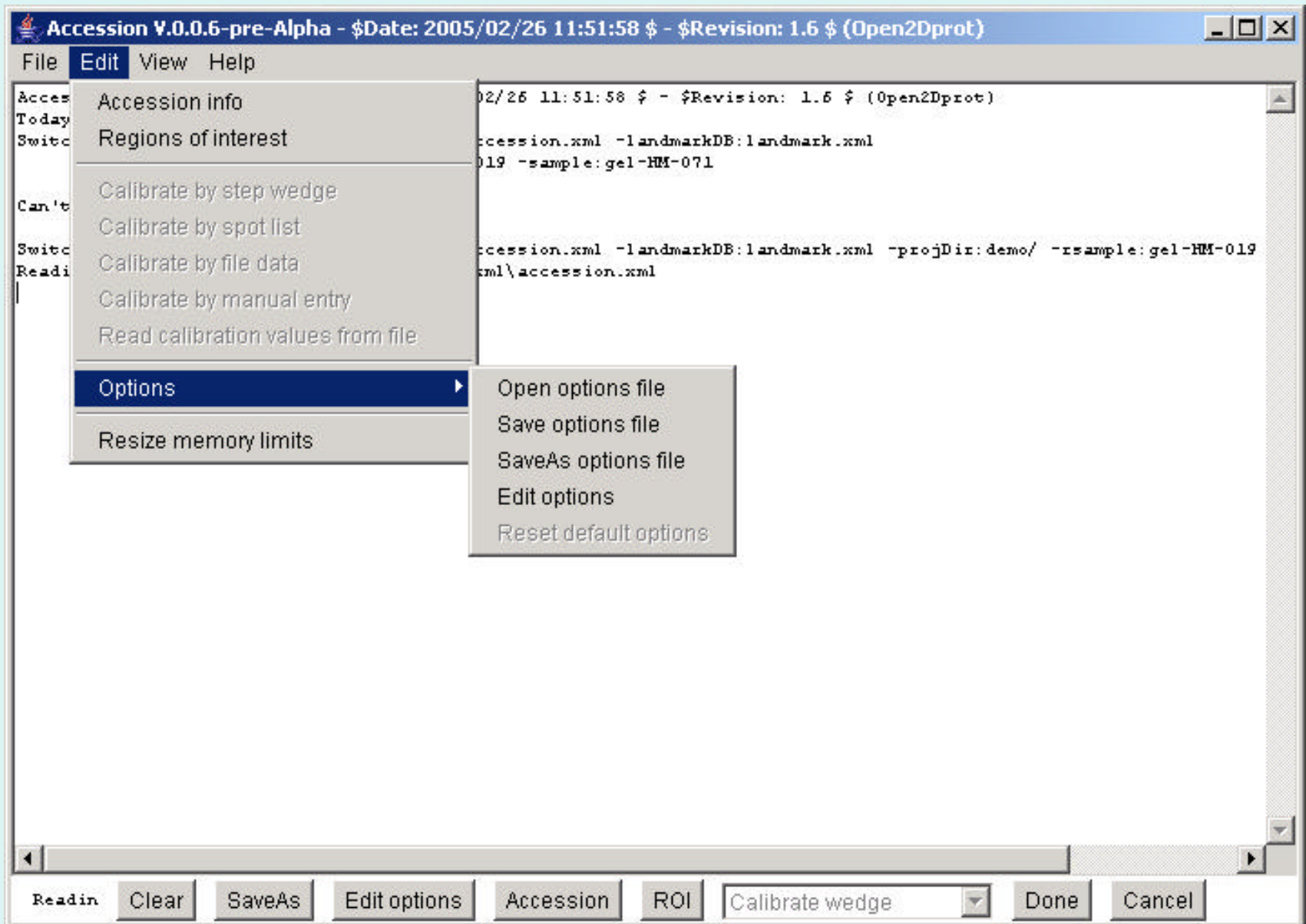
File Menu - Select Current Sample



File Menu - Update From Web Server



Edit Menu



Edit Menu - Accession

Accession edit sample [Sample] 03/01/05 12:52:28

File Edit Help

Accession fields

'Sample' is the sample name for the entry in the accession file. It is also the name of the image file.
'Rsample' is the Reference sample name for the entry in the accession file. It is also the name of the image file.
'PatientNbr' is the patient number associated with the Sample.

| | |
|------------------------------|---|
| Sample | gel-HM-071 |
| Rsample | gel-HM-019 |
| PatientNbr | 34 |
| Study | HEME MALIG-ALL,LYMPHOID (SCAN 1 OF 3) |
| ExperimentDate | T18 MONTHS |
| CultureReagent | CULT #2 |
| AmpholyteAndGelGradientRange | 3:10,5-20% |
| IntervalBeforeLabeling | 0 HRS |
| LabelingIsotope | H3 |
| DurationLabel | 2 HRS |
| DurationExposure | 96 HRS |
| Camera | VIDICON-AUTO,28MM,F8,76CM |
| Investigator | LESTER |
| wedgeCalList | .05,.20,.35,.50,.66,.80,.95,1.10,1.25,1.41,1.56,1.72,1.87,2.02,2.17 |
| wedgeGrayList | 028 051 075 098 118 138 155 169 183 192 200 208 215 225 229 |
| cwx1 | 6 |
| cwx2 | 450 |
| cwy1 | 68 |
| cwy2 | 503 |
| calCWx1 | 0 |
| calCWx2 | 0 |
| calCWy1 | 0 |
| calCWy2 | 0 |
| PixWidth | 512 |
| PixHeight | 512 |

Use log Reset defaults Done Cancel

Edit Menu – Accession editing options

Accession edit sample [Sample] 03/01/05 13:08:34

File Edit Help

- Assign current Rsample entry to this sample
- Clear image computing window ROI entry
- Clear calibration wedge ROI entry

| | |
|------------------------------|---|
| Sample | gel-HM-071 |
| Rsample | gel-HM-019 |
| PatientNbr | 34 |
| Study | HEME MALIG-ALL,LYMPHOID (SCAN 1 OF 3) |
| ExperimentDate | T18 MONTHS |
| CultureReagent | CULT #2 |
| AmpholyteAndGelGradientRange | 3:10,5-20% |
| IntervalBeforeLabeling | 0 HRS |
| LabelingIsotope | H3 |
| DurationLabel | 2 HRS |
| DurationExposure | 96 HRS |
| Camera | VIDICON-AUTO,28MM,F8,76CM |
| Investigator | LESTER |
| wedgeCalList | .05,.20,.35,.50,.66,.80,.95,1.10,1.25,1.41,1.56,1.72,1.87,2.02,2.17 |
| wedgeGrayList | 028 051 075 098 118 138 155 169 183 192 200 208 215 225 229 |
| cwx1 | 6 |
| cwx2 | 450 |
| cwy1 | 68 |
| cwy2 | 503 |

Use log Reset defaults Done Cancel

Edit Menu – Accession New Sample Using Old Sample Information as Template

| Field | Value |
|------------------------------|-------|
| PatientNbr | |
| Study | |
| ExperimentDate | |
| CultureReagent | |
| AmpholyteAndGelGradientRange | |
| IntervalBeforeLabeling | |
| LabelingIsotope | |
| DurationLabel | |
| DurationExposure | |
| Camera | |
| Investigator | |
| wedgeCalList | |
| wedgeGrayList | |
| cwx1 | 0 |
| cwx2 | 511 |
| cwy1 | 0 |
| cwy2 | 511 |
| calCWx1 | 0 |
| calCWx2 | 0 |
| calCWy1 | 0 |
| calCWy2 | 0 |
| PixWidth | 512 |
| PixHeight | 512 |

Use log

Edit Menu – Accession Sample after Template

Accession edit sample [Sample] 03/01/05 12:54:16

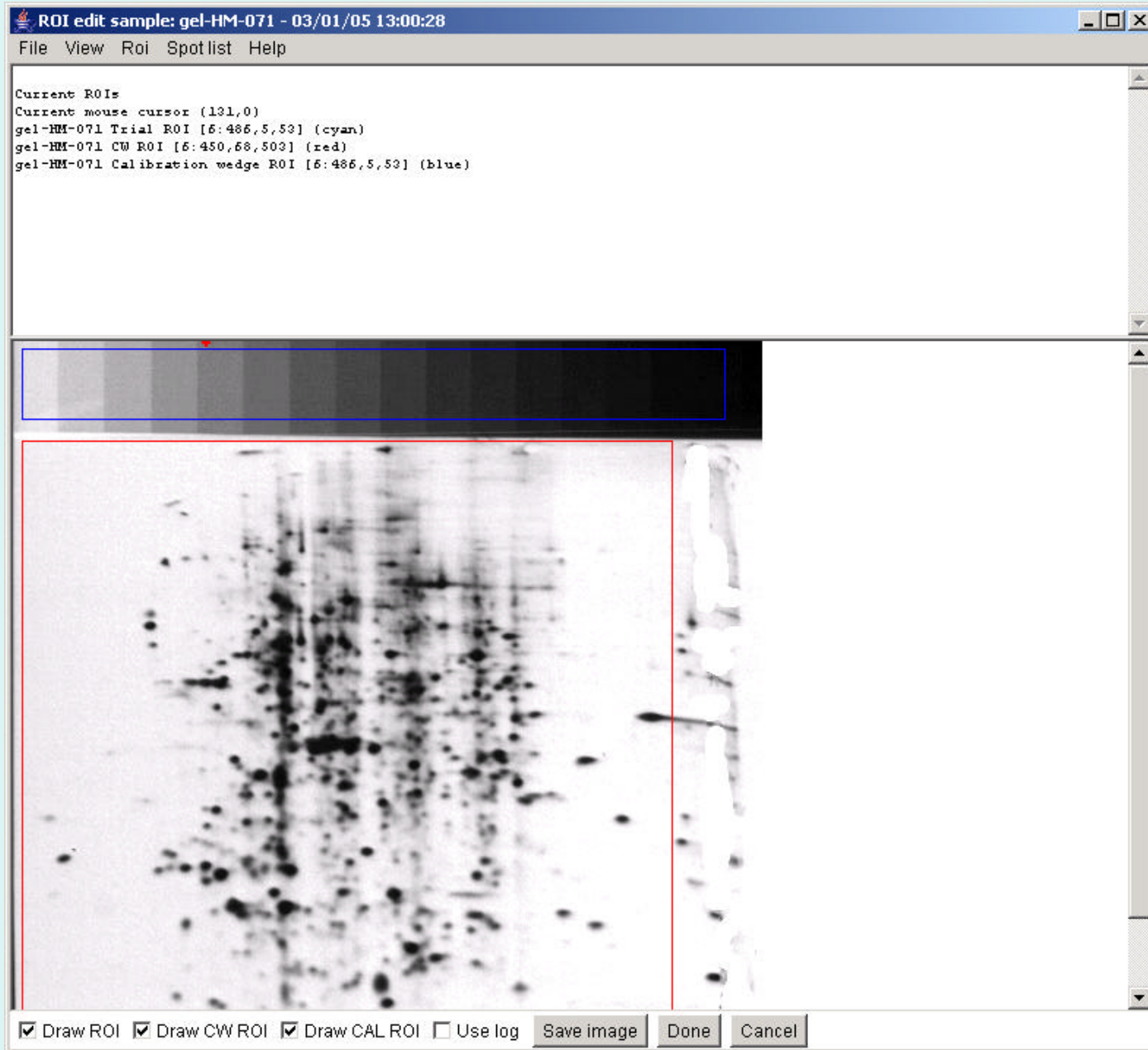
File Edit Help

Using template [gel-HM-019] for Sample [Human-AML]

| | |
|------------------------------|---|
| Sample | Human-AML |
| Rsample | - |
| PatientNbr | 41 |
| Study | HEME MALIG-AML,MYELOID (SCAN 1 OF 3) |
| ExperimentDate | T0 |
| CultureReagent | CULT #2 |
| AmpholyteAndGelGradientRange | 3:10,5-20% |
| IntervalBeforeLabeling | 0 HRS |
| LabelingIsotope | H3 |
| DurationLabel | 2 HRS |
| DurationExposure | 96 HRS |
| Camera | VIDICON-AUTO,28MM,F8,76CM |
| Investigator | LESTER |
| wedgeCallList | .05,.20,.35,.50,.66,.80,.95,1.10,1.25,1.41,1.56,1.72,1.87,2.02,2.17 |
| wedgeGrayList | |
| cwx1 | 0 |
| cwx2 | 511 |
| cwy1 | 0 |
| cwy2 | 511 |
| calCwx1 | 0 |
| calCwx2 | 0 |
| calCwy1 | 0 |
| calCwy2 | 0 |
| PixWidth | 512 |
| PixHeight | 512 |

Use log

Edit Menu – Region Of Interest



Edit Menu – Region Of Interest overlay views

The screenshot shows the 'ROI edit sample: gel-HM-071 - 03/01/05 13:00:28' window. The 'View' menu is open, and the 'WinDump pixel window size' option is selected, opening a sub-menu with the following options:

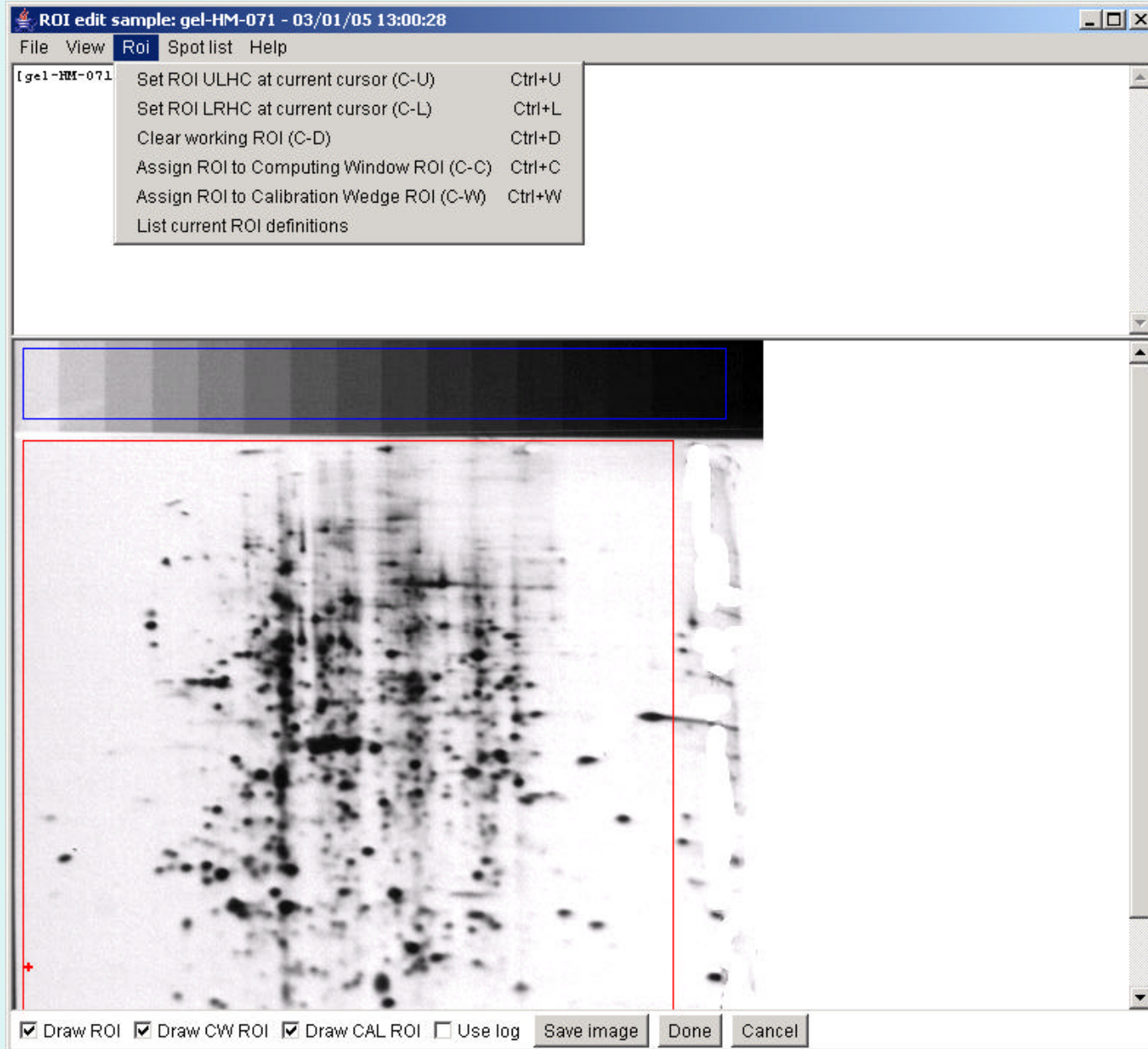
- none
- 3x3
- 5x5
- 7x7
- 9x9
- 11x11
- 13x13
- 15x15
- 17x17
- 19x19
- 21x21

The main window displays a gel image with a red rectangular region of interest (ROI) overlaid. The status bar at the bottom contains the following controls:

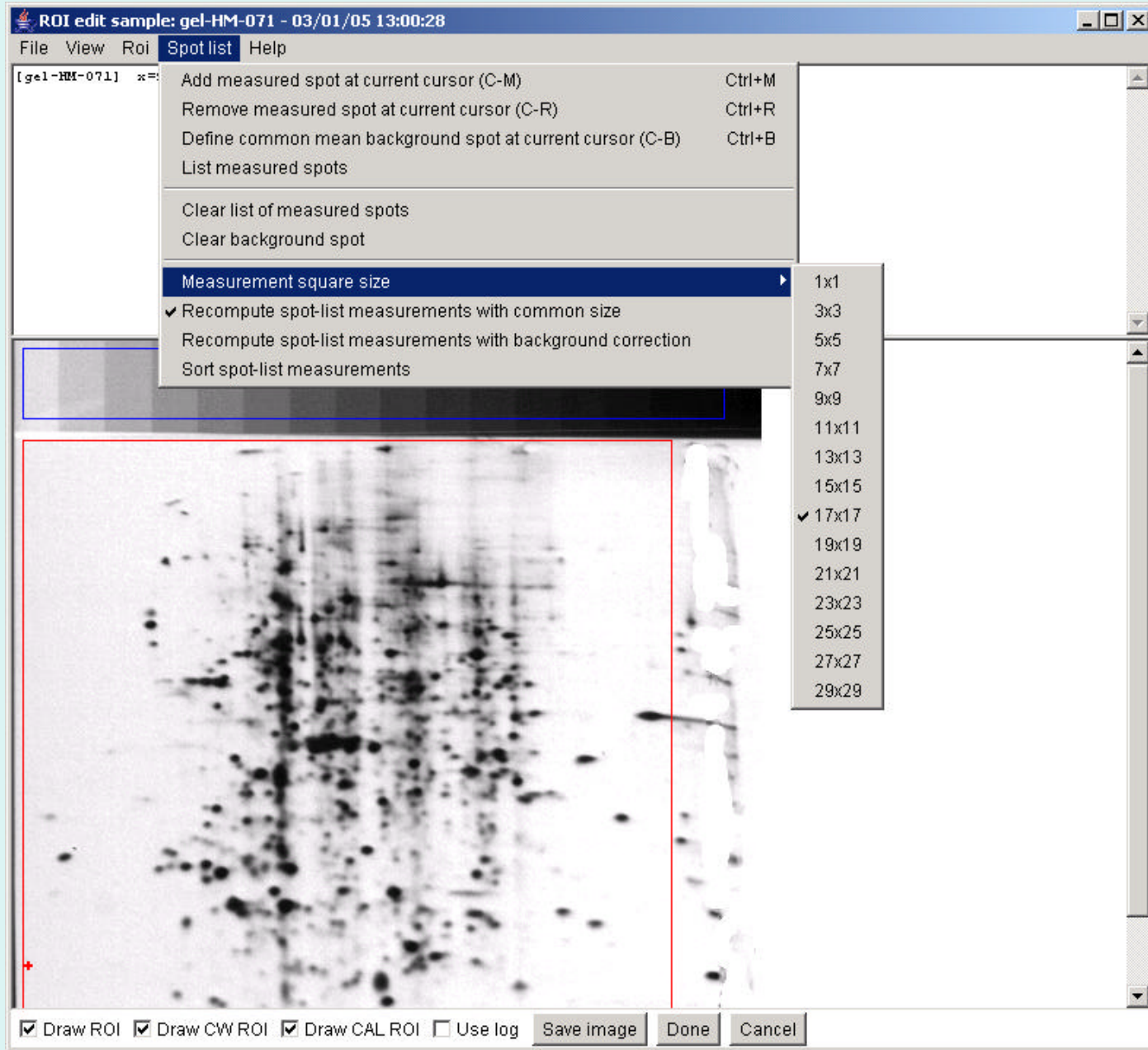
Draw ROI Draw CW ROI Draw CAL ROI Use log Save image Done Cancel

| X | 199 | 200 | 201 |
|-----|-----|-----|-----|
| 195 | 47 | 39 | 39 |
| 196 | 55 | 39 | 31 |
| 197 | 55 | 39 | 39 |
| 198 | 50 | 39 | 39 |
| 199 | | | 39 |
| 200 | | | 39 |
| 201 | 111 | 87 | 111 |
| 202 | 135 | 103 | 119 |
| 203 | 167 | 127 | 151 |

Edit Menu – Region Of Interest commands



Edit Menu – Region Of Interest Spot List



Edit Menu – Calibrate Grayscale – OD, etc.

Calibrate grayscale from step wedge ROI in Sample image gel-HM-071

File View Edit Help

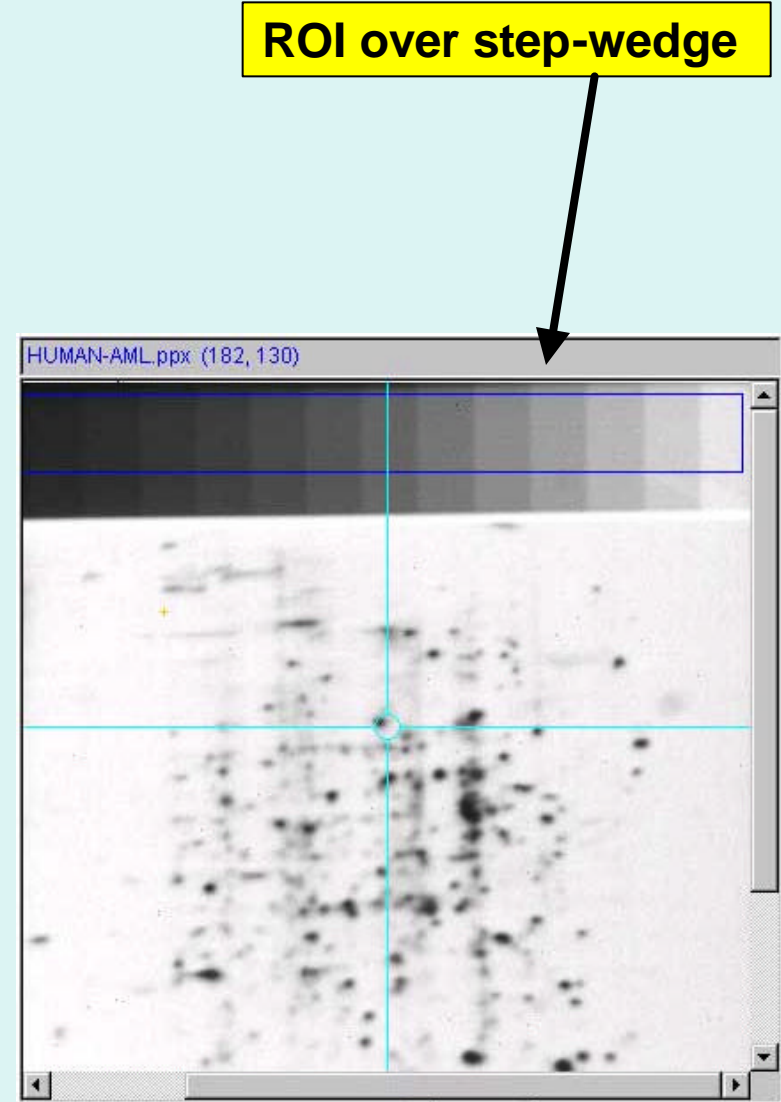
*** UNDER CONSTRUCTION ***

| Calibr. units: | Optical density | Calibr. abbrev.: | od |
|----------------|-----------------|------------------|----|
| Wedge ROI: | [-1:-1, -1:-1] | | |
| Wedge ID#: | <opt. part #> | | |
| Step #1 od: | 0.00 | Gray peak #1: | 0 |
| Step #2 od: | 0.00 | Gray peak #2: | 0 |
| Step #3 od: | 0.00 | Gray peak #3: | 0 |
| Step #4 od: | 0.00 | Gray peak #4: | 0 |
| Step #5 od: | 0.00 | Gray peak #5: | 0 |
| Step #6 od: | 0.00 | Gray peak #6: | 0 |
| Step #7 od: | 0.00 | Gray peak #7: | 0 |
| Step #8 od: | 0.00 | Gray peak #8: | 0 |
| Step #9 od: | 0.00 | Gray peak #9: | 0 |
| Step #10 od: | 0.00 | Gray peak #10: | 0 |
| Step #11 od: | 0.00 | Gray peak #11: | 0 |
| Step #12 od: | 0.00 | Gray peak #12: | 0 |
| Step #13 od: | 0.00 | Gray peak #13: | 0 |
| Step #14 od: | 0.00 | Gray peak #14: | 0 |
| Step #15 od: | 0.00 | Gray peak #15: | 0 |
| Step #16 od: | 0.00 | Gray peak #16: | 0 |
| Step #17 od: | 0.00 | Gray peak #17: | 0 |
| Step #18 od: | 0.00 | Gray peak #18: | 0 |
| Step #19 od: | 0.00 | Gray peak #19: | 0 |
| Step #20 od: | 0.00 | Gray peak #20: | 0 |

Analyze wedge ROI Add peak Delete peak Refresh peak table Save calibration Use log Done Cancel

Flicker - Calibrating Grayscale with a ND Step-Wedge

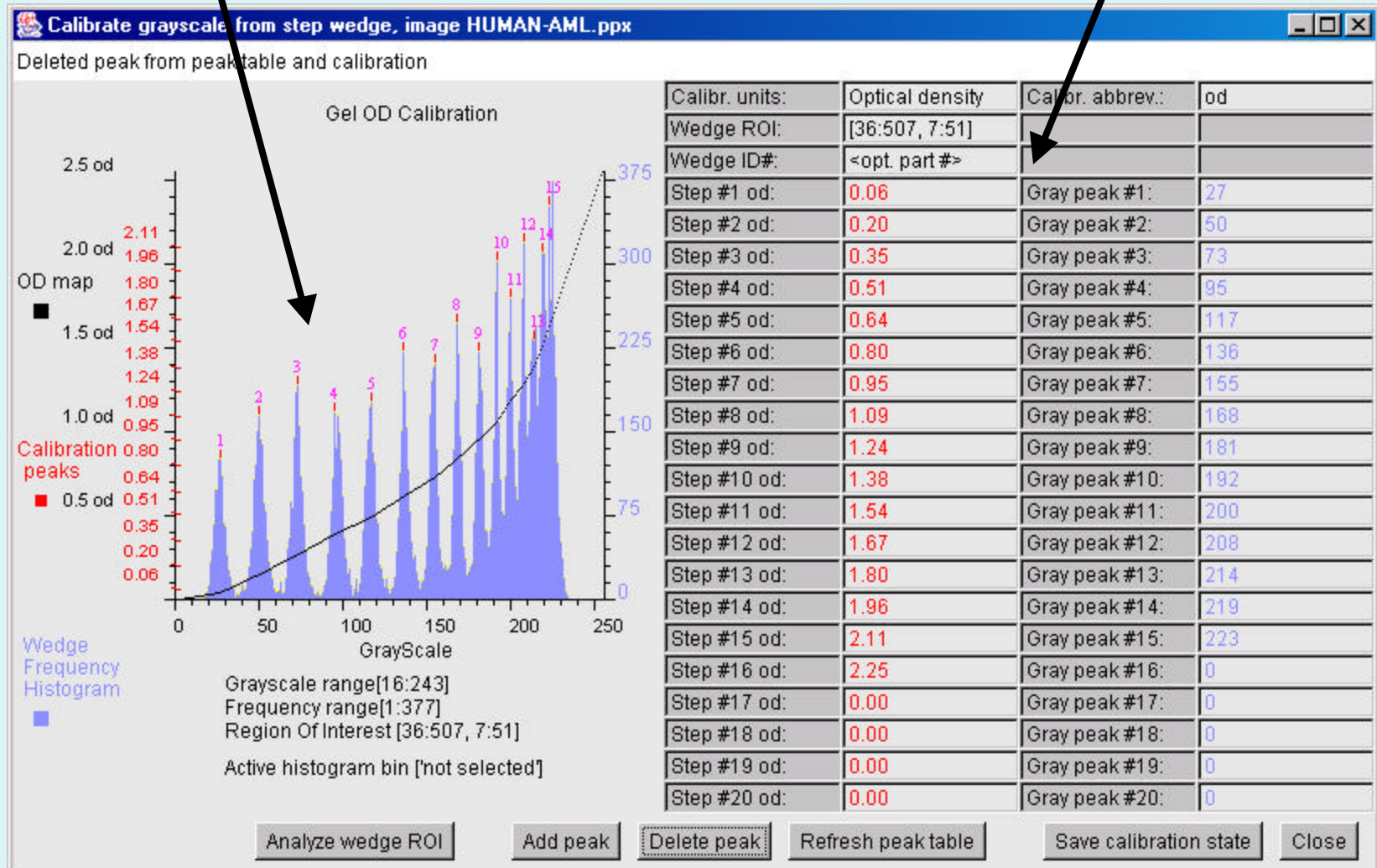
1. The ND step wedge must be scanned with the image and the corresponding OD values known for each step
2. A region of interest (ROI) is overlaid on the step step-wedge
3. The ND wedge calibration wizard is invoked to analyze the data and estimate the calibration



Flicker - Calibrating Grayscale from ND Wedge Data

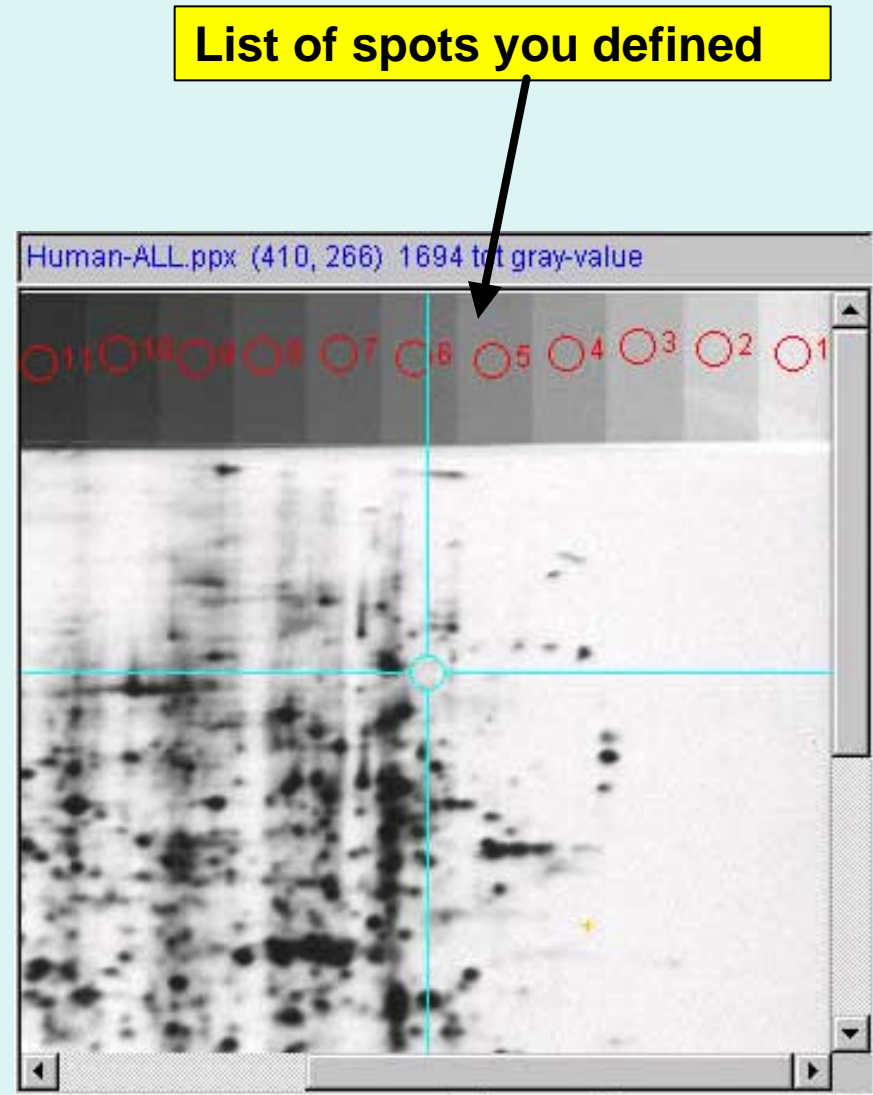
ROI histogram, peaks found and extrapolated calibration curve

OD vs gray-peaks table



Flicker- Calibrating Grayscale with a Spot List of Calibrated Data

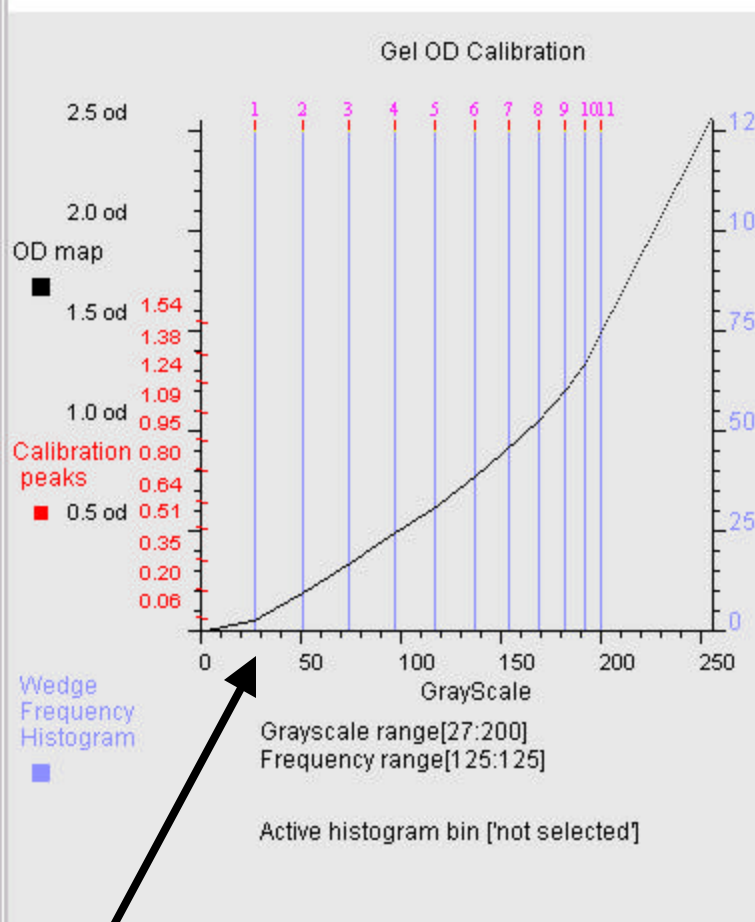
1. The image must contain calibrated regions with known concentrations or corresponding OD values known for each spot
2. You define a set of spots using (C-M) or (ALT-click)
3. The Spot List Calibration wizard is invoked to analyze the data and estimate the calibration



Flicker - Calibrating Grayscale from Spot List Data

Calibrate grayscale from spot list, image Human-ALL.ppx

OD vs gray-peaks table



| Calibr. units: | Optical density | Calibr. abbrev.: | od |
|------------------|-----------------|------------------|-----|
| Mean spot values | | | |
| Wedge ID#: | <opt. part #> | | |
| Step #1 od: | 0.06 | Gray peak #1: | 27 |
| Step #2 od: | 0.20 | Gray peak #2: | 51 |
| Step #3 od: | 0.35 | Gray peak #3: | 74 |
| Step #4 od: | 0.51 | Gray peak #4: | 97 |
| Step #5 od: | 0.64 | Gray peak #5: | 117 |
| Step #6 od: | 0.80 | Gray peak #6: | 137 |
| Step #7 od: | 0.95 | Gray peak #7: | 154 |
| Step #8 od: | 1.09 | Gray peak #8: | 169 |
| Step #9 od: | 1.24 | Gray peak #9: | 182 |
| Step #10 od: | 1.38 | Gray peak #10: | 192 |
| Step #11 od: | 1.54 | Gray peak #11: | 200 |
| Step #12 od: | 1.67 | Gray peak #12: | 0 |
| Step #13 od: | 1.80 | Gray peak #13: | 0 |
| Step #14 od: | 1.96 | Gray peak #14: | 0 |
| Step #15 od: | 2.11 | Gray peak #15: | 0 |
| Step #16 od: | 2.25 | Gray peak #16: | 0 |
| Step #17 od: | 0.00 | Gray peak #17: | 0 |
| Step #18 od: | 0.00 | Gray peak #18: | 0 |
| Step #19 od: | 0.00 | Gray peak #19: | 0 |
| Step #20 od: | 0.00 | Gray peak #20: | 0 |

ROI histogram, peaks found and extrapolated calibration curve

Refresh peak table Save calibration state Close

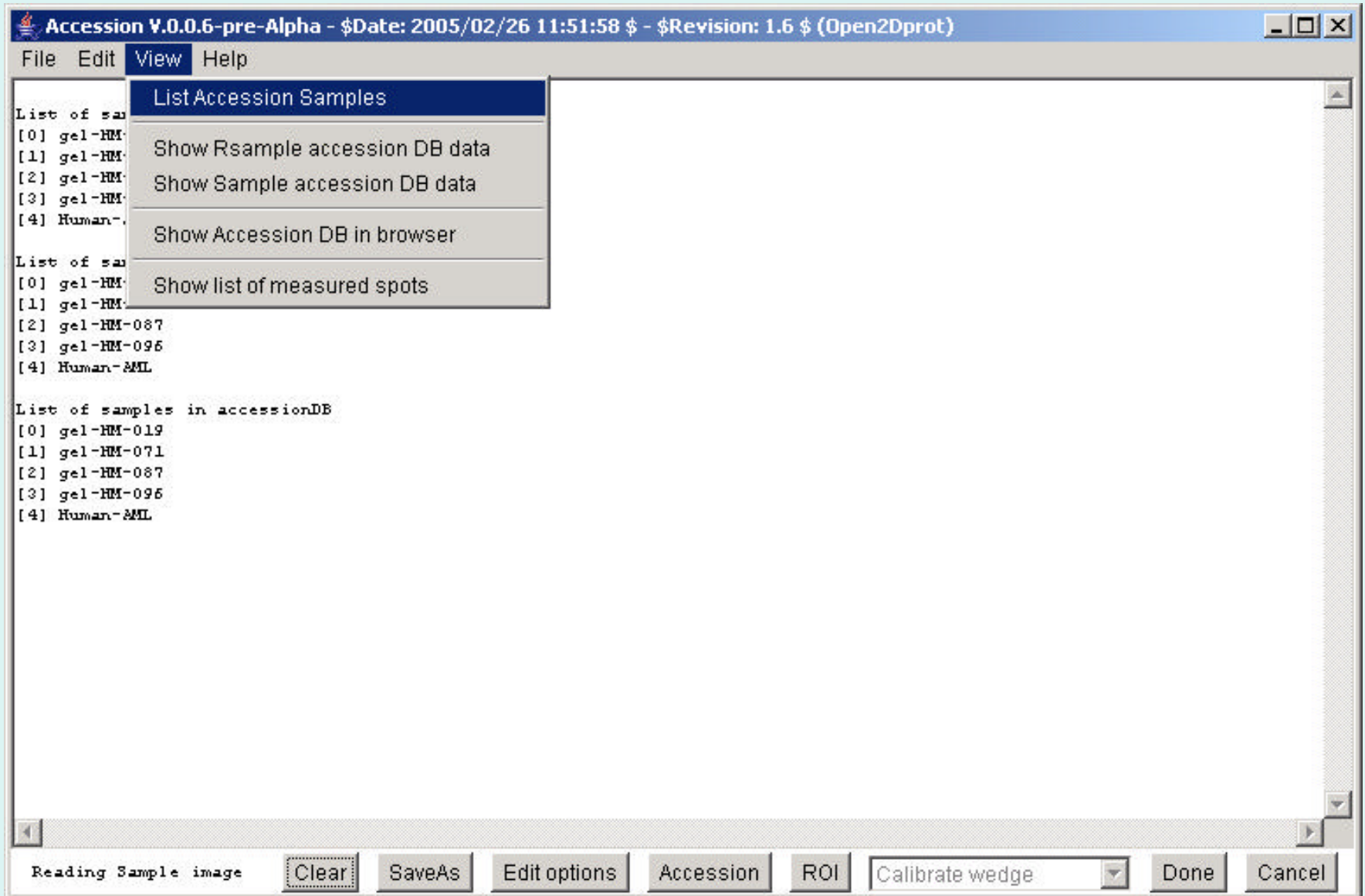
Edit Menu - command line options

Enter sample image and select switch options

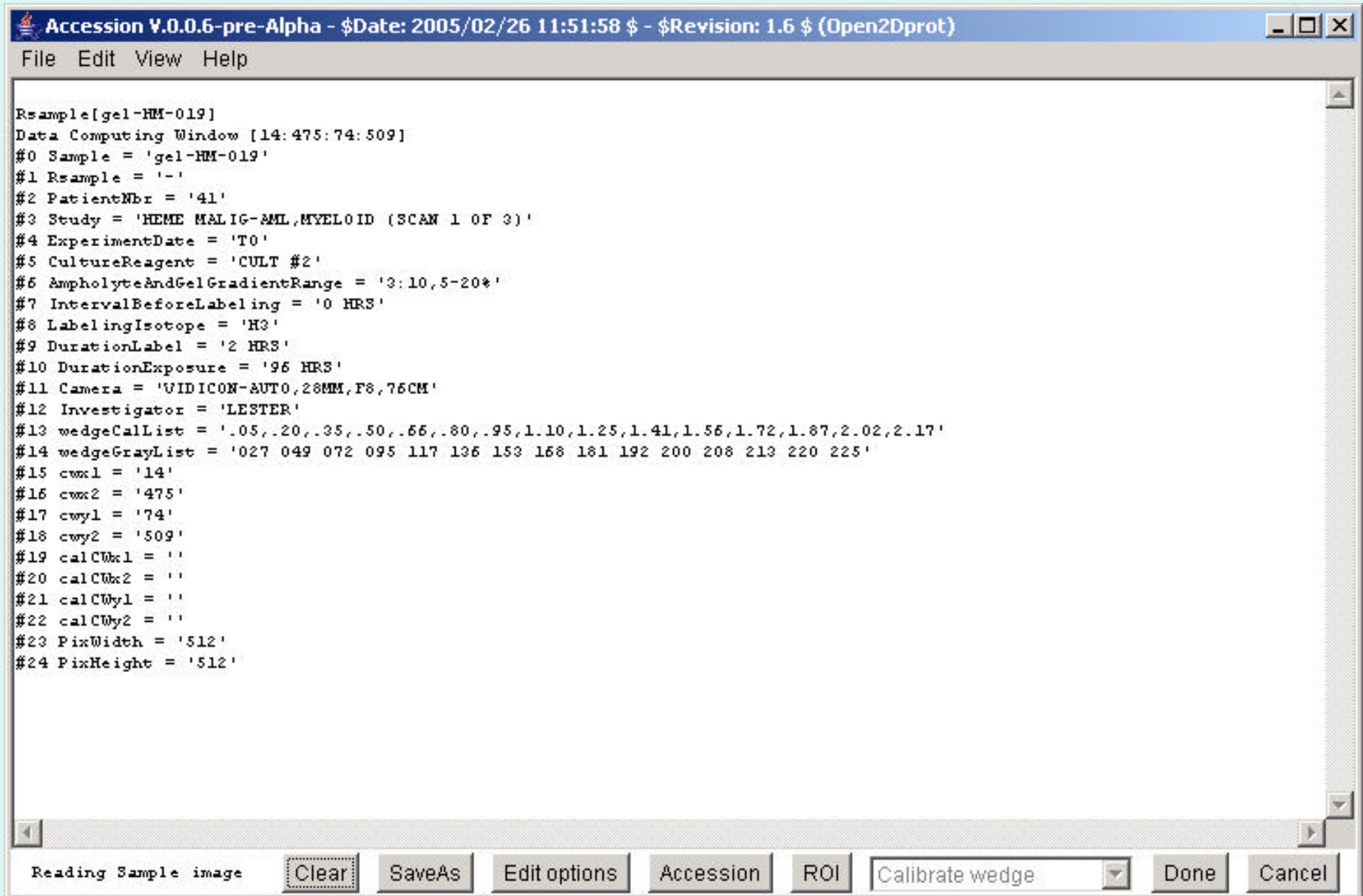
Change the startup parameters, then press 'Set new options' button to save them.
At that point, you can press 'Pair spots' to pair the Rsample and Sample with
the new parameters. You may also enter new Rsample and Sample data file names
and/or edit switch options and threshold sliders.

| | |
|--|----------------------|
| <input checked="" type="checkbox"/> -accessionFile | accession.xml |
| <input checked="" type="checkbox"/> -backupDatabases | --- |
| <input type="checkbox"/> -debugBits | 0 |
| <input type="checkbox"/> -default | --- |
| <input checked="" type="checkbox"/> -demo | --- |
| <input type="checkbox"/> -dtd | --- |
| <input checked="" type="checkbox"/> -inputFormat <input type="text" value="X"/> | X |
| <input checked="" type="checkbox"/> -projDir Project directory <input type="button" value="Browse dir"/> | demo\ |
| <input type="checkbox"/> -propertiesFile Properties file <input type="button" value="Browse file"/> | Accession.properties |
| <input checked="" type="checkbox"/> -rsample Rsample file <input type="button" value="Browse file"/> | gel-HM-019 |
| <input checked="" type="checkbox"/> -sample Sample file <input type="button" value="Browse file"/> | gel-HM-071 |
| <input type="checkbox"/> -timer | --- |
| <input type="checkbox"/> -update <input type="text" value="program"/> | program |

View Menu



View Menu - Show Current Sample Acc DB Data



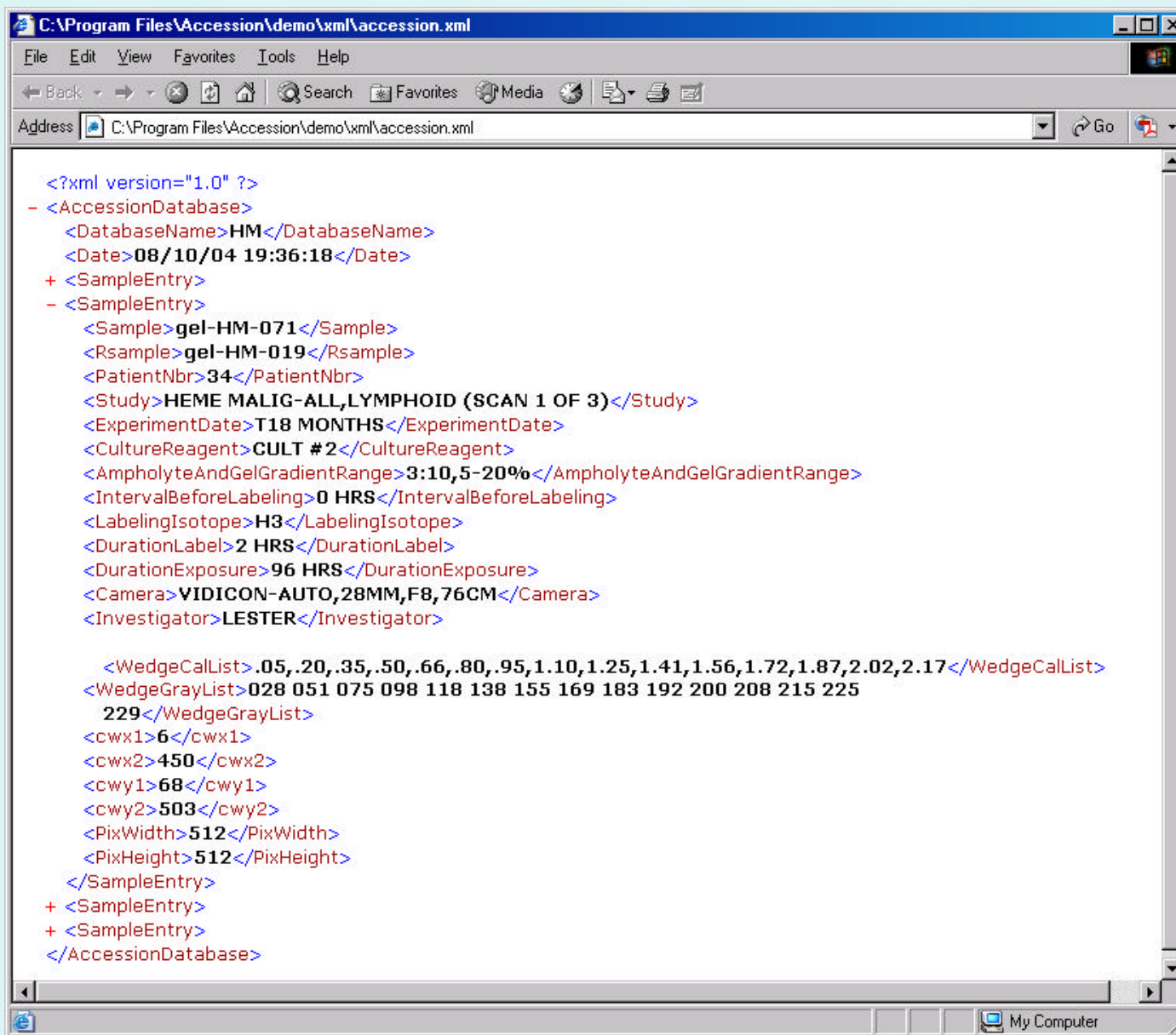
Accession V.0.0.6-pre-Alpha - \$Date: 2005/02/26 11:51:58 \$ - \$Revision: 1.6 \$ (Open2Dprot)

File Edit View Help

```
Rsample[gel-HM-019]
Data Computing Window [14:475:74:509]
#0 Sample = 'gel-HM-019'
#1 Rsample = '-'
#2 PatientNbr = '41'
#3 Study = 'HEME MALIG-AML,MYELOID (SCAN 1 OF 3) '
#4 ExperimentDate = 'T0'
#5 CultureReagent = 'CULT #2'
#6 AmpholyteAndGelGradientRange = '3:10,5-20*'
#7 IntervalBeforeLabeling = '0 HRS'
#8 LabelingIsotope = 'H3'
#9 DurationLabel = '2 HRS'
#10 DurationExposure = '96 HRS'
#11 Camera = 'VIDICON-AUTO,28MM,F8,76CM'
#12 Investigator = 'LESTER'
#13 wedgeCalList = '.05,.20,.35,.50,.66,.80,.95,1.10,1.25,1.41,1.56,1.72,1.87,2.02,2.17'
#14 wedgeGrayList = '027 049 072 095 117 136 153 168 181 192 200 208 213 220 225'
#15 cwx1 = '14'
#16 cwx2 = '475'
#17 cwy1 = '74'
#18 cwy2 = '509'
#19 calCwx1 = ''
#20 calCwx2 = ''
#21 calCwy1 = ''
#22 calCwy2 = ''
#23 PixWidth = '512'
#24 PixHeight = '512'
```

Reading Sample image

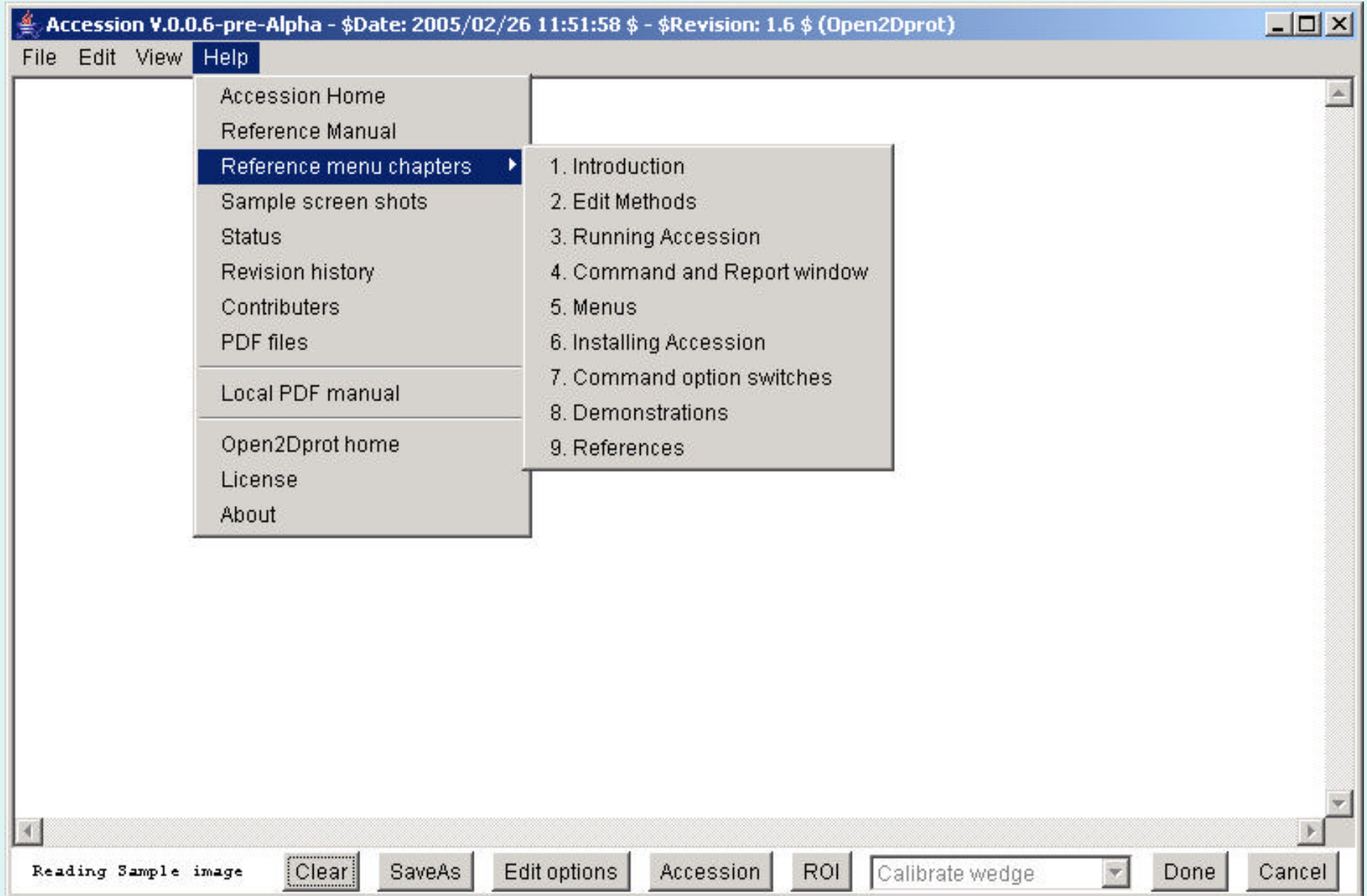
View Menu - XML Accession DB in Browser



```
<?xml version="1.0" ?>
- <AccessionDatabase>
  <DatabaseName>HM</DatabaseName>
  <Date>08/10/04 19:36:18</Date>
  + <SampleEntry>
  - <SampleEntry>
    <Sample>gel-HM-071</Sample>
    <Rsample>gel-HM-019</Rsample>
    <PatientNbr>34</PatientNbr>
    <Study>HEME MALIG-ALL,LYMPHOID (SCAN 1 OF 3)</Study>
    <ExperimentDate>T18 MONTHS</ExperimentDate>
    <CultureReagent>CULT #2</CultureReagent>
    <AmpholyteAndGelGradientRange>3:10,5-20%</AmpholyteAndGelGradientRange>
    <IntervalBeforeLabeling>0 HRS</IntervalBeforeLabeling>
    <LabelingIsotope>H3</LabelingIsotope>
    <DurationLabel>2 HRS</DurationLabel>
    <DurationExposure>96 HRS</DurationExposure>
    <Camera>VIDICON-AUTO,28MM,F8,76CM</Camera>
    <Investigator>LESTER</Investigator>

    <WedgeCalList>.05,.20,.35,.50,.66,.80,.95,1.10,1.25,1.41,1.56,1.72,1.87,2.02,2.17</WedgeCalList>
    <WedgeGrayList>028 051 075 098 118 138 155 169 183 192 200 208 215 225
      229</WedgeGrayList>
    <cwx1>6</cwx1>
    <cwx2>450</cwx2>
    <cwy1>68</cwy1>
    <cwy2>503</cwy2>
    <PixWidth>512</PixWidth>
    <PixHeight>512</PixHeight>
  </SampleEntry>
  + <SampleEntry>
  + <SampleEntry>
</AccessionDatabase>
```

Help Menu



Summary

- Accession is an open-source sample accessioning Java program freely available at <http://open2dprot.sourceforge.net/Accession>
- Useful for adding sample experiment information, regions of interest and grayscale calibration (if available).
- It will be used as one of the step [1] alternative modules in the analysis pipeline in the Open2Dprot project at <http://open2dprot.sourceforge.net>