

Minutes EDNA Plugin Developers' Workshop
ESRF MD-1-21 seminar room
October 22nd – October 24th

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Participants

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Introduction

A part from serving as a discussion forum around the project and the tutorials, the workshop turned out to be very useful for discussing the future directions of the EDNA project. From the point of writing these minutes, the results of these discussions are perhaps the most important topic to be communicated. This does not mean that the tutorials were not important, they proved to be very useful for sharing the knowledge on how to participate in the EDNA developments in general and in particular on how to develop a plugin. The minutes of the discussions and the tutorials can be found in the Annexes :

- The workshop followed approximately the agenda which can be found in Annexe 1.
- The resume of the workshop instruction can be found in Annexe 2.
- Many discussions took place during the tutorials and before starting to discuss the future developments, see Annexe 3 for a resume.
- About half of the available time for the workshop was used for the two tutorials :
 - Labelit, Annexe 4
 - ISPyB, Annexe 5
- Finally there were some discussions around an EDNA GUI, see Annexe 6.

Future development discussions

The starting point of these discussions was the current status of the EDNA prototype as presented by Olof :

- We have so far succeeded to develop :
 - A plugin framework, a testing framework and a data model framework
 - A very robust prototype that works and which can easily be modified / extended
 - A development practices scheme : code review, coding convention etc
 - A project web / wiki / development server which is easily accessible
 - A starting point for the documentation
- What we are lacking :
 - More developers !
 - More documentation

After some discussions, three clear possible future directions were identified (see Figure 1):

1. The release of the prototype with another name. It was agreed that the prototype has been proved to be sufficiently stable to be used, and it is already in "production use" (I.e. incorporated in the beamline control software CBASS, see Annexe 6) at the NSLS.
2. Improvements of the generic data model to allow inclusion of XDS indexing and integration. Although the prototype contains a generic data model, it is not sufficiently generic for allowing easy integration of the XDS indexing and integration plugins. Therefore more work is needed for improving the generic data model.
3. Development of non-MX EDNA applications : Both at Diamond and at the ESRF there is a strong interest for using the EDNA framework for tomography applications. Especially the plugin framework, the data model framework and the possibility of clustering parallel execution are felt to be of great usefulness for tomography data reduction.

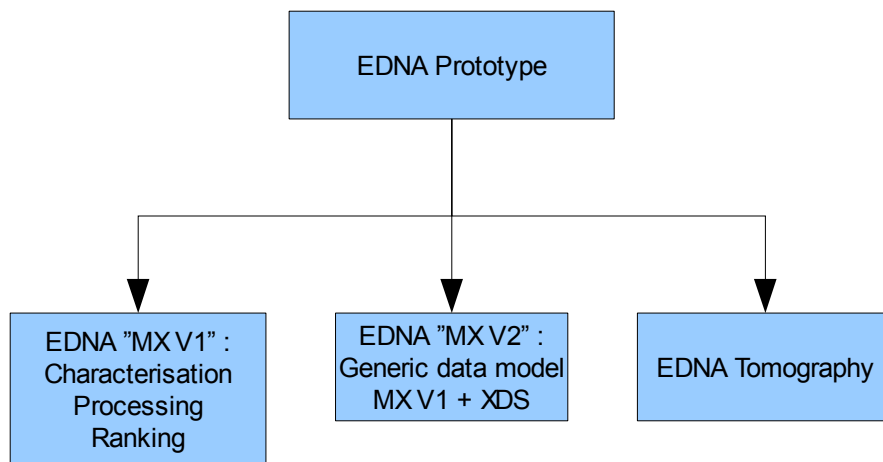


Figure 1 : The three possible future EDNA development directions.

It was agreed that not only the prototype could be served as base for the three future directions, but that there were many EDNA kernel developments that could be shared between these three (kernel, testing framework etc). The three different directions would have their own data models and plugins. Marie-Françoise suggested to split the current data model into pieces that could serve as bases for the MX V1, MX V2 and Tomography (however not for the prototype in order to avoid potential regressions).

Suggested future EDNA Project hierarchy

After some further discussions we agreed that the following project hierarchy could be a possible solution for sharing common features at the same time as the different directions could each have their own specific developments:

- Libraries
- Prototype
- Kernel
 - Common data model
 - Kernel source
 - Testing framework
 - Common plugins with specific data models that could be shared between different versions, e.g. MOSFLM, BEST, RADDPOSE etc. would be used both by MX V1 and MX V2
- MX Version 1
 - V1 "generic" data model
 - Applications / Plugins
- MX Version 2
 - V2 truly generic data model
 - Applications / Plugins
- Tomography
 - Tomography "generic" data model
 - Applications / Plugins

Suggested development plan

The following development plan will be submitted to the EDNA executive committee for approval. The idea is that all the proposed developments will be managed in parallel, i.e. once approved the new developments will start at the same time :

The EDNA prototype

The EDNA prototype will be continued to be developed and maintained. No major changes will be introduced neither to the framework nor to the data model. The following plugins / functionalities will gradually be added:

- Labelit indexing (see Annexe 4)
- ISPyB connection (see Annexe 5)
- MOSFLM post processing
- Pointless
- SCALA
- Ranking
- and possibly more.

As outline below in the section for EDNA MX V1, once MX V1 is ready for release the development and support for the prototype will be discontinued. This could mean that some of the suggested plugins above will be directly implemented in MX V1 instead of the prototype.

EDNA Kernel

The common data model will be refurbished and the project hierarchy will be changed as outlined in section "Suggested future EDNA Project hierarchy" (previous page). Some of the prototype execution plugins with specific data models which will be shared between MX V1 and MX V2 will be reused as kernel plugins, e.g. the MOSFLM, BEST and RADDOSSE plugins.

EDNA MX Version 1

This version will basically be the prototype using the new EDNA kernel with major changes to the prototype "characterisation" data model. All functionality of the prototype will be implemented (i.e. all plugins will be reused). Once the EDNA MX version 1 is released the support for the prototype will be discontinued.

EDNA MX Version 2

This version will use the new EDNA kernel. The generic data model of the prototype will be improved in order to integrate XDS indexing and integration. All features of EDNA MX V1 will be implemented. Once EDNA MX V2 is released the support and maintenance of EDNA V1 will be discontinued.

EDNA Tomography

The tomography version will also be based on the EDNA kernel. It will have its own (generic) data model and plugins for tomography applications.

Development time-scales

The time-scale is very difficult to estimate, during the workshop the only one proposed was the 6 months estimation by Olof for developing the new kernel and the MX Version 1. The estimation of MX Version 2 and Tomography has been made by Olof after the workshop:

- Prototype : continuous development and maintenance till MX Version 1 is released.
- Kernel and MX Version 1 : at least 6 months of development from now
- MX Version 2 : probably between 6 months and a year from now
- Tomography : at least 6 months of development of a tomography prototype

Development resources

This is the current status concerning development resources :

- Prototype and new kernel : Marie-Françoise, Karl and Olof
- Plugins : Marie-Françoise, Karl, Olof, John (Labelit) and Johan (Scala)
- MX Version 1 : Marie-Françoise, Karl and Olof
- MX Version 2 new generic data model : Gleb, Sandor, Pierre and Peter would be responsible for the new design. Marie-Françoise and Olof will participate as well in the discussions in order to assure compatibility with the new EDNA kernel common data model.
- MX Version 2 XDS plugin : Gleb, Sandor and Pierre
- Tomography : Mark and Olof

EDNA Publication

We all agreed that it would be a good idea to publish the EDNA developments. Sandor suggested to make a start by dividing up an article in parts which were distributed to participants in the workshop, like the article for the DNA developments were distributed. Olof suggested instead that Marie-Françoise and himself write a draft which is later circulated for comments.

The best time for publication is probably around the release of EDNA MX Version 1.

Next Meeting

We discussed briefly (during the dinner...) the possibility of a follow-up meeting :

- We agreed that there's no need to organise a full EDNA meeting in December as suggested in the prototype demonstration meeting in June.
- Manfred Weiss suggested to Olof before the workshop to arrange the next developers' meeting in Hamburg. A possibility would therefore be to organise a new developers' meeting, possibly combined with an EDNA full meeting, in Hamburg in about 6 months.

Annexe 1 : Agenda

Wednesday October 22nd

- 14:00 - 15:30 : Session 1: Introduction, presentation of participants, presentation of the current status of the prototype, how to develop an EDNA plugin: overview
- 15:30 - 16:00 : Coffe break
- 16:00 - 18:00 : Session 2: Testing framework, start of Labelit and ISPyB plugins

Thursday October 23rd

- 09:00 - 10:30 : Session 3: Data propagation
- 10:30 - 11:00 : Coffee break
- 11:00 - 12:30 : Session 4: Development process: from Use Case to Code Review
- 12:30 - 14:00 : Lunch
- 14:00 - 15:30 : Session 5: Free
- 15:30 - 16:00 : Coffee break
- 16:00 - 18:00 : Session 6: Feedback discussions, future development plans, involvements
- 18:00 - 20:00 : Transport to the restaurant "Chez le Per' Gras"
- 20:00 - : Dinner

Friday October 24th

- 09:00 - 10:30 : Session 7: Parallel execution
- 10:30 - 11:00 : Coffee break
- 11:00 - 13:00 : Session 8: Workshop wrap-up

Annexe 2 : Workshop Introduction

After some initial struggle to allow the participants to connect to the ESRF Guest wifi network, Olof opened the workshop and gave a short history of the EDNA project together with his vision of the goals with this workshop :

- Give clear explanations on :
 - What is an EDNA plugin and how it works
 - How to develop new plugins
 - How to participate as a developer in the EDNA collaborations
- Develop in common at least two plugins :
 - Labelit indexing plugin
 - ISPyB plugin
- Serve as a discussion forum around the EDNA project :
 - Improvements to the framework and development practices
- Define together possible development plans :
 - Names (of new developers) attached to new plugins...

After this introduction each participant presented themselves and their opinion on the EDNA collaboration and the prototype.

In the second session a couple of topics were discussed before the plugin tutorial started :

- Johan wanted to know why EDNA was programmed in Python and not in Java. Olof answered that the choice of Python was mainly a legacy from the DNA project and the choice of the BLISS group to use Python for their developments. Therefore the EDNA kernel and the plugins are programmed in Python.
- Even though the code base of EDNA is in Python, EDNA could be executed in a Java virtual machine using the Jython interpreter. This has not been tested with the prototype and there are probably some issues that needs to be solved before running the prototype in Jython.
- We discussed briefly the problem of supporting several versions of the same third-party software, e.g. supporting versions 7.0.1, 7.0.2, 7.0.3 and 7.0.4 for MOSFLM. The main problem is the data for the testing framework, if we support all versions we must supply test data from each version. Another solution is to support only the latest versions in the tests. No clear consensus were reached.
- Romeu asked why the AALib generateDS function was not used for generating the data bindings. Olof answered that the reason is that some extra functions needed by EDNA was added to the data bindings, e.g. parseString. Additional functionality will probably be added in the future, for example a “compare” method which can compare two data binding objects and have some tolerance when comparing float values, e.g. accept that “0.25” and “0.2500001” are equal.

Annexe 3 : Discussions

During and after the tutorials we discussed many points related to the current status of the EDNA project. The questions related to the two tutorial plugins can be found in their respective Annexe (Labelit : Annexe 3 and ISPyB Annexe 4).

Plugin execution validation tests

Gleb said that in general it will be impossible to directly compare the XML output of a plugin with a reference XML file : different versions of underlying third-party programs can produce slightly different results which are not significant but will make XML comparison fail. Another problem highlighted by Olof is that the resulting XML often contain paths to result files, which will not be the same if executed on a different system. Therefore, the meaning of success of a plugin must be more carefully defined and the execution tests must be modified to more intelligently analyse the results of a plugin execution test.

Data binding scripts

Olof pointed out that the current scripts for generating the data bindings for the plugin specific data models are not very easy to use. They must be moved from the EDNA directory utils / datamodel to their respective plugins. The script must also be improved in order to be more simple to use.

Use Cases

Olof also suggested that a new form for formulating the Use Cases must be found. The Use Cases are necessary for the EDNA developments, however their present incarnation on the Wiki must be simplified.

Developers' documentation

John found that the developers' documentation on the Wiki was in general very good, in particular it allowed him to set up Enterprise Architect for starting a new data model. However, he lacked documentation on how to do the actual modelling. Olof agreed that this part of the documentation needs to be expanded. Mark suggested to use 'videos', he pointed out that the preparation of a video demonstrating a particular feature is often faster than trying to explain the feature using screen-shots and text.

Licence

The licence for the kernel is currently GNU Public Licence version 3. No one disagreed to continue to use this licence. Peter pointed out that any work at Global Phasing would not be released under GPL, but as no work is foreseen at Global Phasing that would involve the kernel this should not be an obstacle.

Anonymous subversion access

We agreed that the access to the EDNA subversion repository could be made publicly readable, however the write access should of course be limited to EDNA developers. [Before changing the EDNA subversion server the EDNA executive committee will be asked to give their approval].

Bugzilla access

On the other hand we agreed to continue to block the EDNA bugzilla server from public access, i.e. only developers will have read (and write) access to the EDNA bugzilla server.

EDNA Portal discussion forum

Peter pointed out a potential weakness with the EDNA Portal discussion forum compared with mailing lists: if someone starts a new thread potentially interested people are not automatically notified. Olof pointed out that there might be a solution by subscribing to the discussion forum RSS feed, the icon for subscription can be found in the lower right corner of the forum page. Olof also suggested to remove the forum “child boards” since there are very few discussions and the topic of a discussion server the same purpose. Another problem with the discussion forum is the limited range of available “avatars”... Karl reported that he couldn't update his avatar. [Olof has temporarily disabled the use of avatars till these problems has been sorted out].

EDNA wiki discussion pages

We agreed that these pages are well suited for discussing the layout and contents of the corresponding wiki page, however they are much less suited for discussing e.g. a Use Case, the discussion forum should be used in this case.

Problem with the setDataInput method

In the current implementation all plugins must define a “setDataInput” method. We agreed that it would be better to allow plugins deriving directly from EDPlugin to not have to implement this method, but to keep the restriction for plugin derived from EDPluginExec and EDPluginControl. (A problem was encountered when executing the plugin unit tests when the setDataInput was missing in the tested plugin, the number of successes and failures were both set to zero.)

Project management software

Romeu suggested to use the “Mylyn” Eclipse plugin for enabling integrated project management in the Eclipse IDE. Olof supports this idea, it might be necessary though to upgrade the bugzilla server as the current one installed on www.edna-site.org (version Version 2.22-debian1) does not seem to work with the Mylyn plugin.

Annexe 4 : The Labelit plugin tutorial

The following documentation were used for the tutorial :

- http://www.edna-site.org/wiki/index.php/How_to_develop_an_EDNA_plugin
- http://www.edna-site.org/wiki/index.php/How_to_test_an_EDNA_plugin
- http://www.edna-site.org/wiki/index.php/Tutorial_on_developing_an_XDS_spot_search_plugin

The Labelit program is different to both MOSFLM and XDS because it relies almost entirely to access all relevant input parameters in the image headers. It will therefore be difficult to use the EDNA design criteria to not rely on the image header information. Another limitation when using Labelit is that it can only work with one or two images, and in the latter case only if the starting oscillation angle between the two images is greater than four degrees.

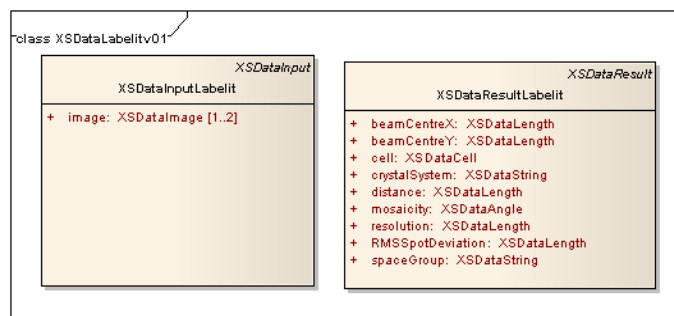
Use Case

The tutorial for writing a Labelit indexing plugin started by jointly defining a simplified Use Case :

- This plugin should run Labelit.
- Required input
 - A list of paths to one or two diffraction images.
- Required output
 - Beam centre, distance, mosaicity, Cell, crystal system, space group, resolution, RMS spot deviation
- Checks before execution
 - Max two images at least 4 degrees apart.

Data model

We then defined a specific data model:



We then proceeded to generate the data bindings:

- Scripts for generating the data binding : <http://www.edna-site.org/svn/trunk/edna/prototype/utis/datamodel/generateXSDataLabelitv01.sh>
- Specific Labelit data binding generated by this script : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/plugins/XSDataLabelitv01.py>

Test data and test code

- Test configuration file : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/tests/data/XSConfiguration.xml>
- Test input data file : http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/tests/data/XSDataInputLabelit_reference.xml

We then proceeded by writing the Labelit plugin unit test :

- The plugin unit test suite : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/tests/testsuite/EDTestSuitePluginUnitLabelitv01.py>
- The plugin execute test suite : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/tests/testsuite/EDTestSuitePluginExecuteLabelitv01.py>
- The plugin unit test case with the method testSetDataInput : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/tests/testsuite/EDTestCasePluginUnitLabelitv01.py>
- The plugin execute test : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/tests/testsuite/EDTestCasePluginExecuteLabelitv01.py>

The Labelit plugin

We then started writing the Labelit plugin, starting with the method setDataInput :

<http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginLabelit-v0.1/plugins/XSDataLabelitv01.py>

These test methods and the first version of the plugin were committed as revision #575.

We discussed briefly the error handling as described on the wiki :

http://www.edna-site.org/wiki/index.php/How_to_develop_an_EDNA_plugin#Developing_the_plugin_-_tutorials

Annexe 5 : The ISPyB Plugin Tutorial

Use Case

We agreed in the workshop that there will be a need of several IPSyB plugins, initially at least two :

1. One plugin that can store the characterisation results into the ISPyB "Screening" tables
2. Another plugin that can retrieve the ISPyB diffraction plan

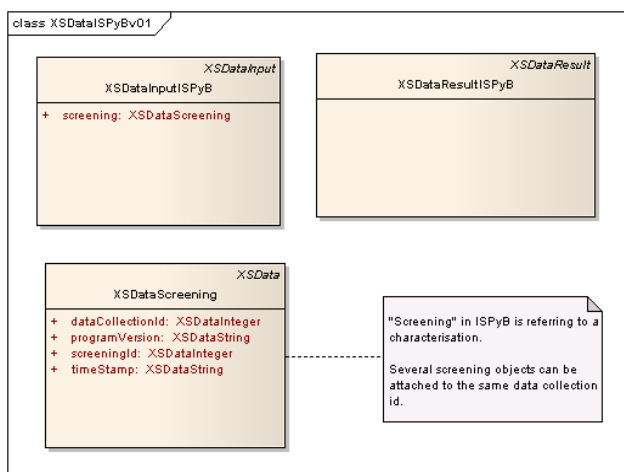
We therefore started by defining the ISPyB plugin folder as a plugin group :

```
$EDNA_HOME/prototype/plugins/EDPluginGroupISPyB-v0.1
```

However, as we would not have the time to develop these two plugins, we agreed to concentrate our efforts on the first one and for the moment simply call the plugin "EDPluginISPyBv01". This name for the plugin that will store the results into the data base will probably be changed as we will need more than one plugin.

- Required input :
 - DataCollectionID.
 - Characterisation results.
 - Configuration: host and port of the server running the DBServer.
- Required output :
 - Success or failure.

Data Model



Data bindings:

- Scripts for generating the data binding : <http://www.edna-site.org/svn/trunk/edna/prototype/utills/datamodel/generateXSDataISPyBv01.sh>
- Specific ISPyB data binding generated by this script : <http://www.edna-site.org/svn/trunk/edna/prototype/plugins/EDPluginGroupISPyB-v0.1/plugins/XSDataISPyBv01.py>

Annexe 6 : EDNA GUI

The following items related to an EDNA GUI were discussed :

- It is essential that non-experts in computing can benefit from the new features in EDNA, e.g. radiation damage. This is difficult without a GUI since it is non-trivial to express the necessary biological / chemical input either on a command line or in an XML input file. Therefore it is urgent to supply these users with a GUI to simplify the use of EDNA.
- John demonstrated a working version of CBASS which has EDNA functionality built-in, e.g. parameters like the completeness and the multiplicity can easily be changed by a user (see screenshot on the following page). EDNA can be launched from CBASS and the EDNA characterisation results can be used for launching data collections. John said that the integration of EDNA was trivial. The feedback he has received so far is that EDNA is a bit worse compared with DNA when it comes to indexing. John thinks that this is due to the fact that DNA installed at the NSLS uses Labelit instead of MOSFLM for indexing.
- Alun had communicated to Olof prior to the workshop that Diamond has plans for running EDNA from the GDA GUI.
- At the ESRF there are plans for developing an EDNA GUI as well for mxCuBE. However, given the present situation concerning the resources for mxCuBE developments, there is a fear that these developments will not be made in the short future. A “mock-up” of a GUI has been created by Elspeth Gordon and Marie-Françoise that will serve as a basis for discussion with the ESRF BLISS group regarding the potential integration of EDNA into mxCuBE (see the following thread in the EDNA discussion forum: http://www.edna-site.org/joomla/index.php?option=com_fireboard&Itemid=3&func=view&catid=16&id=13#13)
- Marie-Françoise and Olof suggest to develop a simple GUI based on the Eclipse Rich Client Project (RCP) framework. The idea is to develop Eclipse RCP plugins which match the EDNA plugins and provide a simple application for running EDNA.

CBASS

File Edit Tools Comments Help

Collect Setup Pucks Canes

	Start	End	Width	Time	File Prefix	NumStart	Distance	Wavelength
1	65.0	113.3	1.05	43.002	x296	0	543.05	1.1000
2								
3								
4								

Goniostat Omega Kappa Phi

Move 91.0000 0.0000 0.0000

Set Relative Zero -> 0.0 0.0 0.0

Set Relative Zero To Current Position

Detector Status Idle 0

Detector Distance 200.0 Move

Edge Resolution 2.52 Move

Detector Tilt 0.0000 Move

1.90 Å
2.52 Å

Collect Data Collect Strategy (EDNA) Open Shutter Close Shutter Home Pause On Beam Dump Clear Collection Clear Top Row Pause Count Abort

File: /home/pxuser/cbass_test/ref-x296_1_002.img CBASS Ready

Command: Group... skinner PxID... px04-4010

EDNA Input Parameter:
 Completeness 0.9900
 I/Sigma 2.0000
 Multiplicity auto
 Resolution auto
 Apply Close

```

Strategy : Best : 7.90 7.25 97.0 1976.3 119.6 16.5 15.0 1.21 5.0 0.00
Strategy : Best : 7.25 6.73 96.0 1264.8 121.9 10.4 9.8 1.11 7.6 0.00
Strategy : Best : 6.73 6.31 99.0 928.0 130.7 7.1 6.9 1.07 10.6 0.00
Strategy : Best : 6.31 5.96 100.0 736.6 142.2 5.2 5.1 1.05 14.0 0.00
Strategy : Best : 5.96 5.67 99.0 616.1 148.8 4.1 4.1 1.04 17.6 0.00
Strategy : Best : 5.67 5.41 99.0 546.1 161.0 3.4 3.3 1.03 21.2 0.00
Strategy : Best : 5.41 5.19 100.0 515.3 169.1 3.0 3.0 1.03 23.6 0.00
Strategy : Best : 5.19 4.99 100.0 481.2 182.5 2.6 2.6 1.02 27.1 0.00
Strategy : Best : 4.99 4.81 100.0 441.2 188.7 2.3 2.3 1.02 30.8 0.00
Strategy : Best : 4.81 4.65 100.0 399.8 199.9 2.0 2.0 1.02 36.3 0.00
Strategy : Best : 12.00 4.65 98.0 1265.6 160.0 7.9 7.6 1.09 8.8 0.00
Strategy :
EDApplicationPrototype-v1.0.0::Runtime: 29.2395579815 [s]
spacegroup = P3 mosaicity = 0.75 resolutionHigh = 4.65 cell_a = 86.009 cell_b = 86.009 cell_c = 156.4334 cell_alpha = 90.0 cell_beta = 90.0 cell_gamma = 120.0 status = ok
dna Strategy results: Start=65.0 End=113.3 Width=1.05 Time=43.002 Dist=543.05
collection_dist 543.05
CBASS>

```

group	px id	xtal id	file template	sweep	# images	tot exp. time	timestamp	
skinner	px04-4010	Standard Project	x296	x296	0	2	10	27-OCT-2008 10:45
spacegroup = P3 mosaicity = 0.75 resolutionHigh = 4.65 cell_a = 86.009 cell_b = 86.009 cell_c = 156.4334 cell_alpha = 90.0 cell_beta = 90.0 cell_gamma = 120.0 status = ok dna Strategy results: Start=65.0 End=113.3 Width=1.05 Time=43.002 Dist=543.05								

[Termin... [EDNA ... [firewir... [pxuse... [xterm] [pxuser... [pxsys... [xterm] [pxuser... [pxuse... [xterm]

Figure 2 : Screenshot of the EDNA prototype interaction in CBASS