IRootLab Tutorials

2-region Pre-processing example

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# Introduction

This tutorial shows how to pre-process two different mid-IR regions separately, and then merge them together into a single dataset.

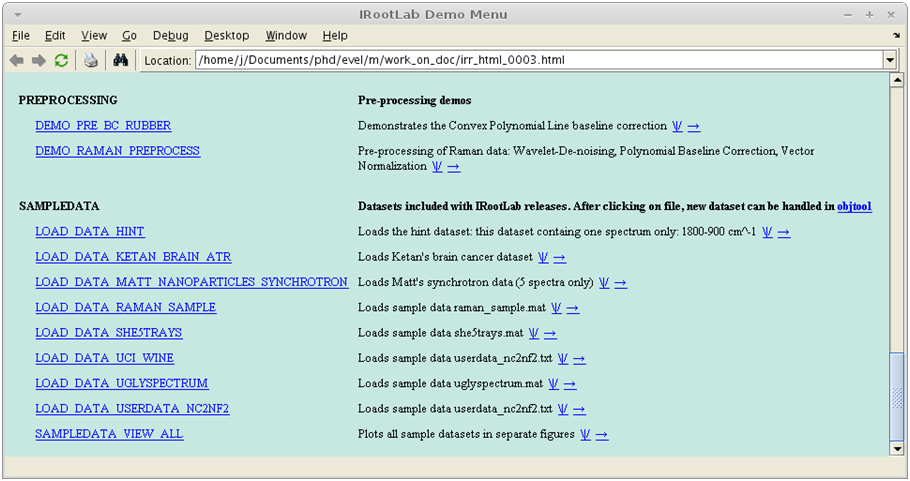
This tutorial uses Matt’s Nanoparticles Synchrotron data, which is shipped with IRootLab. This dataset has spectra initially in the 4000-900 cm-1 region.

# Summary of operations

* Load data
* High region:
  + Cut original to 3700-2800 cm-1 region
  + Rubberband baseline correction
  + Max normalization
* Low region:
  + Cut original to 1800-900 cm-1 region
  + Rubberband baseline correction
  + Amide I peak normalization
* Merge two datasets column-wise

# Load and visualize data

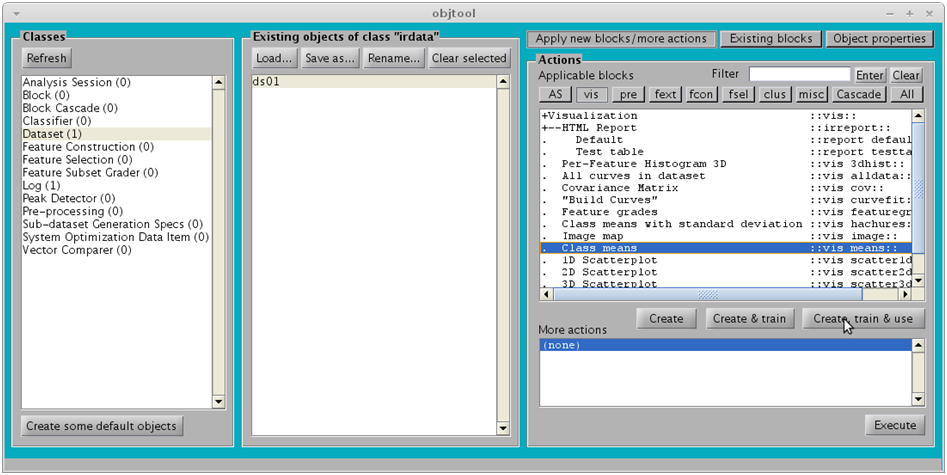
1. At MATLAB command line, enter browse\_demos
2. Click on “LOAD\_DATA\_MATT\_NANOPARTICLES\_SYNCHROTRON”
3. Click on “objtool” to launch objtool



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1. Click on **vis**
2. Click on **Class means**
3. Click on **Create, train & use**

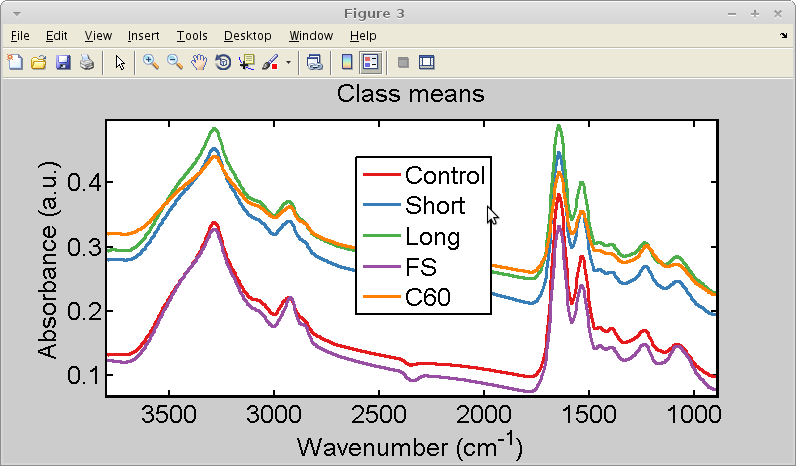


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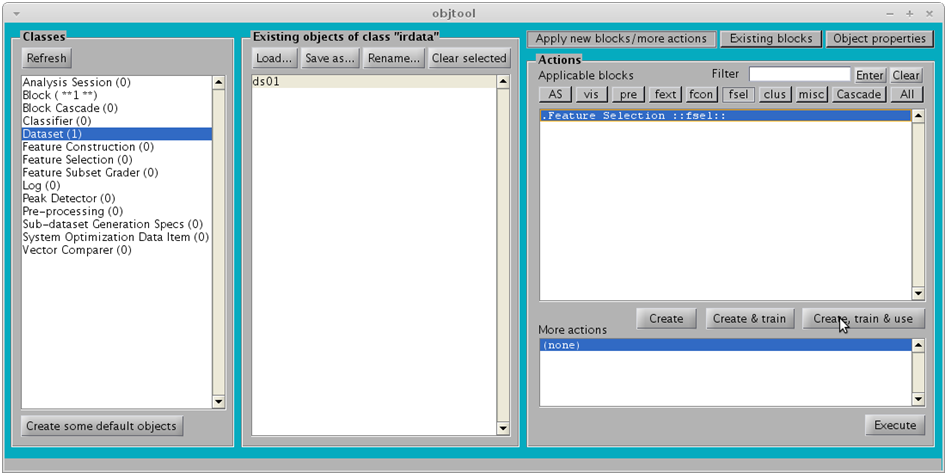
**6**

The following figure should appear:



# High region (3700-2800 cm-1)

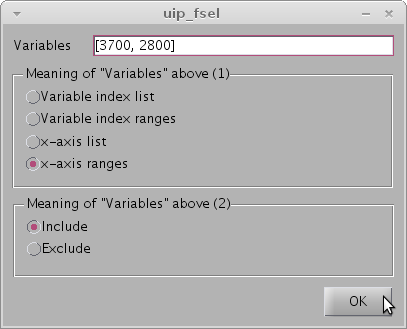
1. Click on **fsel**
2. Click on **Create, train & use**



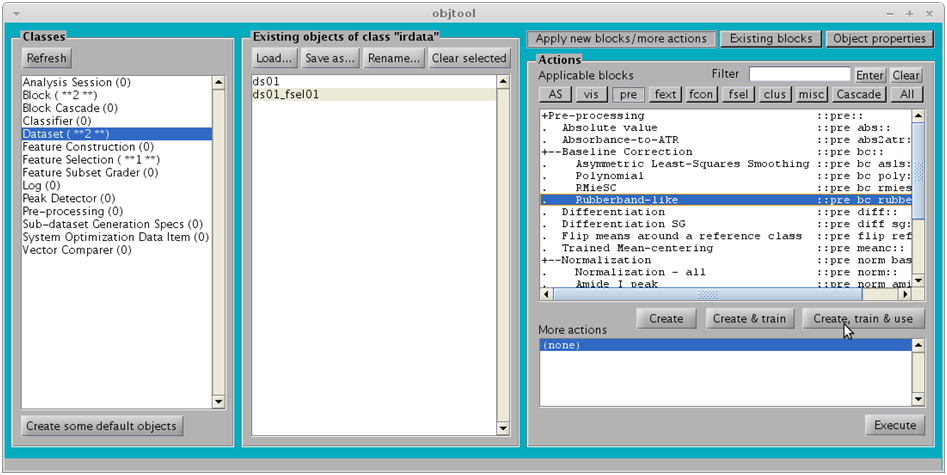
**7**

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1. Specify region **[3700, 2800]** (see below)
2. Click on OK



1. Click on ds01\_fsel01
2. Click on **pre**
3. Click on **Rubberband-like**
4. Click on **Create, train & use**



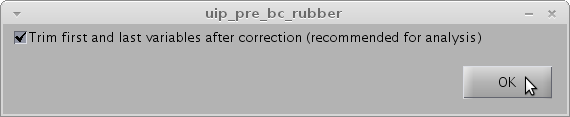
**11**

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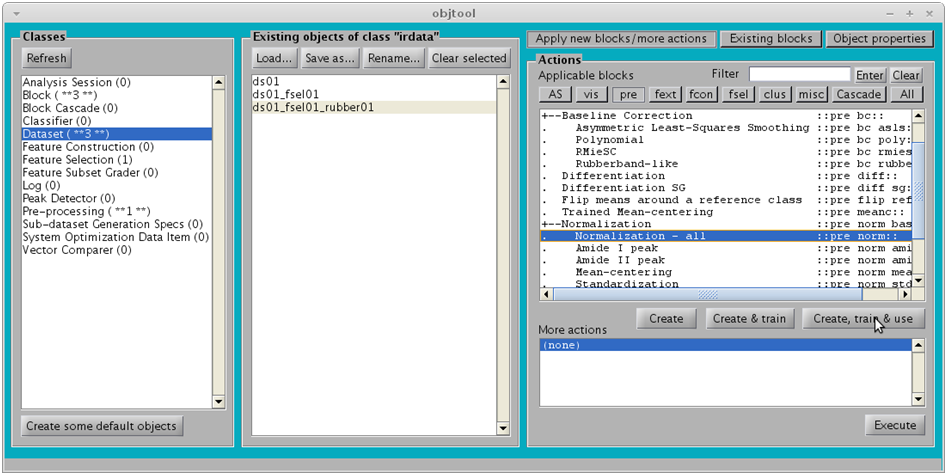
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1. Click on **OK**



1. Click on **ds01\_fsel01\_rubber01**
2. Click on **Normalization-all**
3. Click on **Create, train & use**

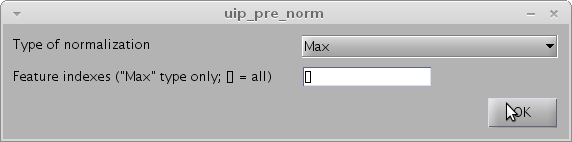


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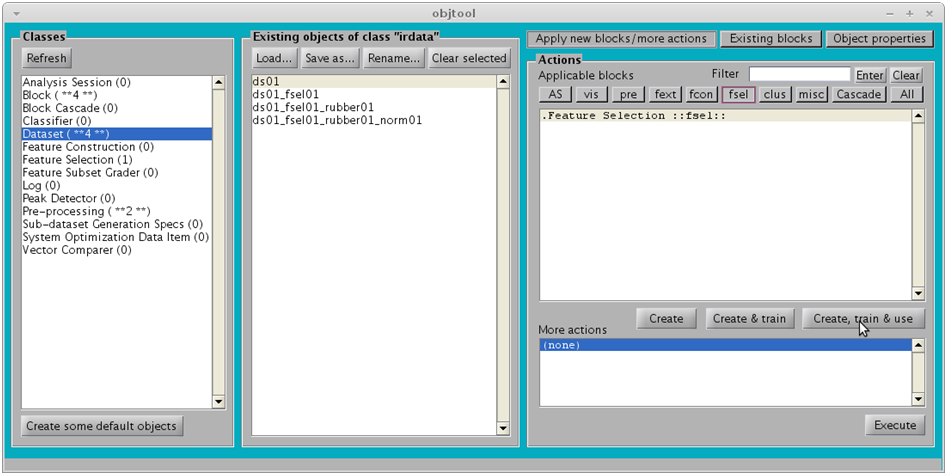
**18**

1. Click on **OK**



# Low region (1800-900 cm-1)

1. Click on **ds01**
2. Click on **fsel**
3. Click on **Create, train & use**

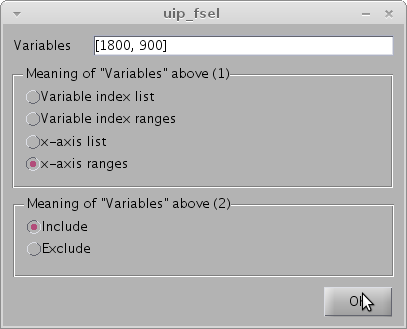


**20**

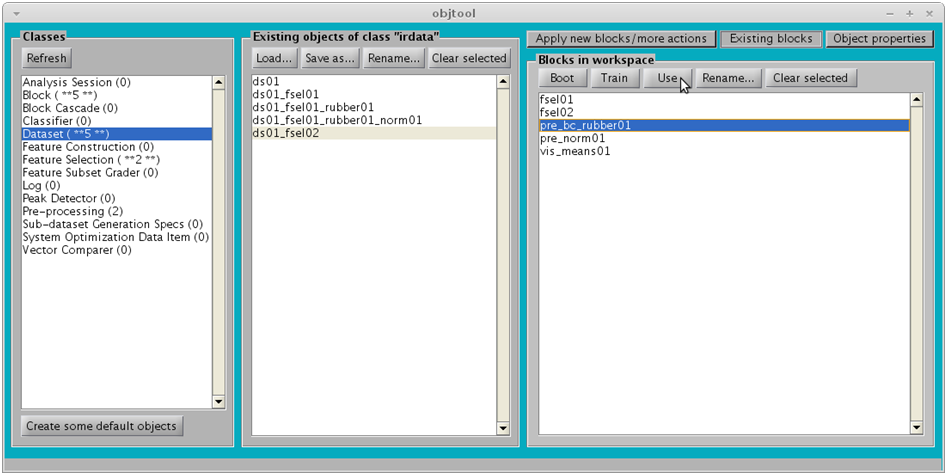
**21**

**22**

1. Accept the default **[1800, 900]** region (see below)
2. Click on OK



1. Click on **ds01\_fsel02**
2. Click on **Existing blocks** (we are going to re-use some blocks)
3. Click on pre\_bc\_rubber01
4. Click on Use



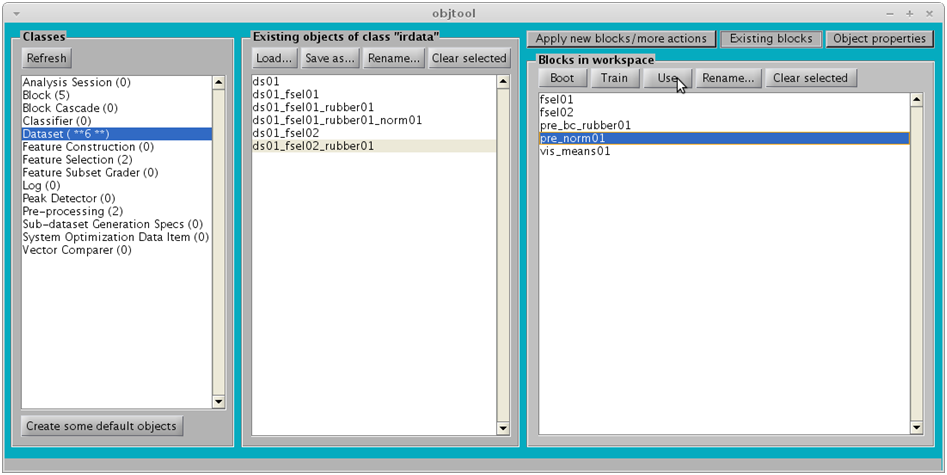
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1. Click on **ds01\_fsel02\_rubber01**
2. Click on pre\_norm01
3. Click on Use



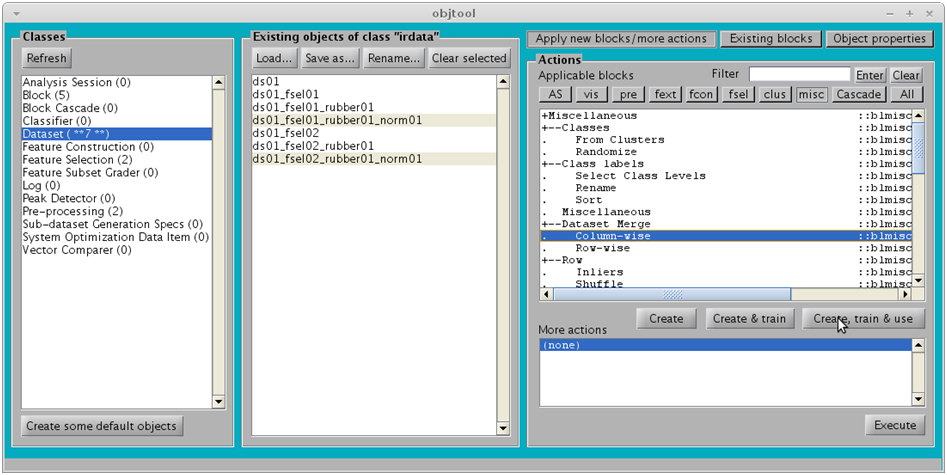
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# Merge two datasets column-wise

1. Hold down the “Ctrl” key to select multiple items
2. Select ds01\_fsel01\_rubber01\_norm01 and ds01\_fsel02\_rubber01\_norm01
3. Click on Apply new blocks/more actions
4. Click on Misc
5. Click on Column-wise
6. Click on Create, train & use



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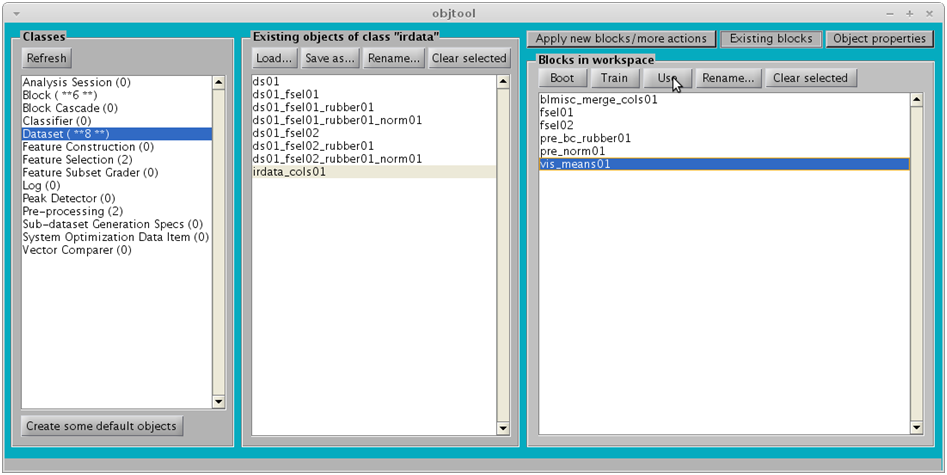
**36**

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# Visualize result

1. Click on irdata\_cols01
2. Click on Existing blocks (we are going to re-use the class means visualization block)
3. Click on vis\_mean01
4. Click on Use



**2**

**1**

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**4**

The following figure should appear:

