RADDOSE-3D GUI User Manual

7 July 2015

Contents

1 Getting Started

I expect this section to contain general information such as why we created RADDOSE-3D GUI and the fact that it's free and open source.

1.1 Why RADDOSE-3D GUI?

1. Improve usability of RADDOSE-3D.
2. Allow comparison of multiple RADDOSE-3D simulations.
3. Free and open source.

1.2 Installing/Running RADDOSE-3D GUI

Here I guess we can talk about how to get the code (git clone ...) and run the right file for the GUI. We'll have to mention that they'll need Python at the very least to run the GUI.

2 Using RADDOSE-3D GUI

This section will form the main bulk of the manual. We need to split this up well so that each individual section can be considered self contained (to a reasonable extent) and is as concise as possible.

2.1 Terminology

We should try to explain the terminology that we'll use regarding the Strategy GUI i.e. what do we mean by:

- Crystal
- Beam
- Strategy
- Experiment

And anything else you might think may not be so obvious.

2.2 Creating an Experiment

2.2.1 Specifying a Crystal

i.e. How to make a crystal object.

2.2.2 Specifying a Beam

i.e. How to make a beam object.

2.2.3 Specifying a Strategy

i.e. How to make a wedge object. (Also explain why a beam is linked to a given strategy).

2.2.4 Running an experiment

Only a brief part about how to run the experiment, that they must supply an experiment name that will be linked to that crystal, beam and strategy combination. Also explain the experiment list window on the right. The summary analysis will be added later.

2.3 Loading Information from a Text File

Explain the different ways that `RADDOSE-3D GUI` can read information from a text file.

2.3.1 Crystal Information

How to read information about a crystal

2.3.2 Beam Information

How to read information about a beam

2.3.3 Experiment

Explain how to load an `RADDOSE-3D` input file and how it creates crystals and beams along with an experiment.

2.4 Analysing Results from Experiments

This section explains how to use the Summary/Output window.

2.4.1 Analyse Results from a Single Experiment

Explains how to view the log, the Experiment Summary and Dose Contours

2.4.2 Compare Results from Multiple Experiments

Explains how to plot the results, save the plots, show summary, save summary table. Also explains the experiment list drop down box and how to load/remove the experiments.

2.5 In-built Help Dialogue

Explain how they can use the help dialogue to help them with their next steps.

3 Glossary

This section is a glossary that will hopefully help users understand what each of the dose terms mean. e.g.

- Dose
- Diffraction Dose Efficiency (DDE)
- Diffraction Weighted Dose (DWD)
- etc.

4 Examples

This section contains worked examples showing typical examples of MX, SAXS and MX comparison experiments.

4.1 Macromolecular Crystallography (MX) Example

Example of using a typical crystal from the PDB

4.2 Small Angle X-ray Scattering Example

Example using a SAXS sample in a quartz capillary

4.3 MX comparison

Example showing how to compare some three loaded experiments.