RnPC: Radionuclide Production Calculations

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Getting Started

RnPC is a graphical user interface (GUI) that can be used for radionuclide production calculations. It is programmed in Matlab. The philosophy behind the program is to be versatile and able to adapt to many different calculations. By modifying the available cross section and target files, the user can calculate the yield and decay products of multiple reactions simultaneously.

Installing the GUI

The GUI can be installed by running a single executable file. The download file can be found at the following address:

- https://github.com/dsfergus/RnPC-public-v1.1
    - Click on the "for_redistribution" folder
    - Download the "MyAppInstaller_web.exe" file
    - Run once installed

This executable file contains all the necessary files for running the GUI. For specific calculations, the user will have to add certain cross-section and target files (see instructions below). Upon execution, the Matlab installer interface will guide the user through the installation process (see Figure 1). This includes downloading and installing the Matlab Runtime Compiler (~757 Mb). This compiler is essential for executing the code.

When specifying a folder for the installation of the RnPC program, the user should select a location that is convenient (i.e. application and data will be stored in this folder, so installing in "My Documents" may be better than in "Program Files" as these files may need to be modified). When selecting the folder for the Matlab Runtime compiler, the "Program Files" folder is adequate as this does not contain any user specified data files.

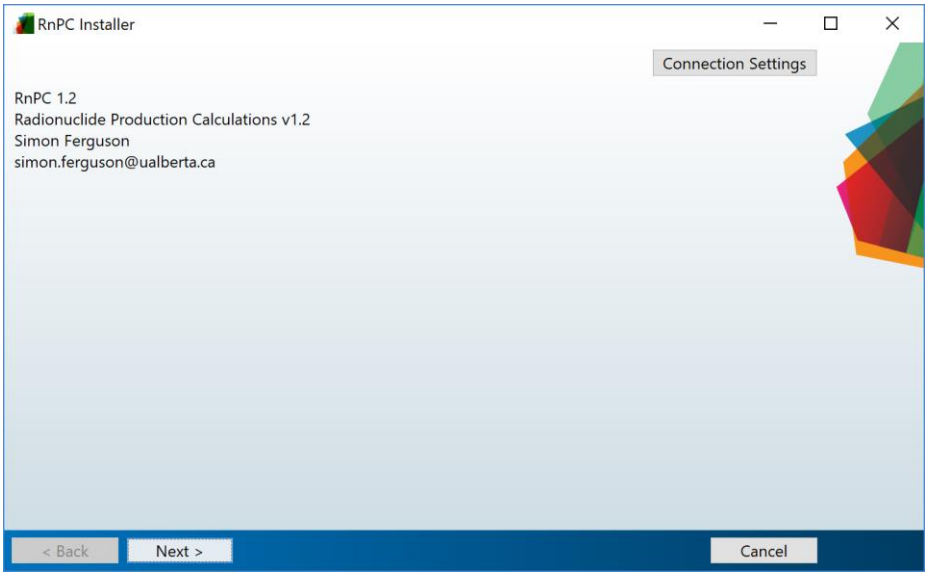


Figure 1: Matlab installer screen which will guide the user through installation after executing "MyAppInstaller_web.exe" file

Upon finishing installation, the program can be executed by running the RnPC.exe file in the application sub-folder of the install directory.

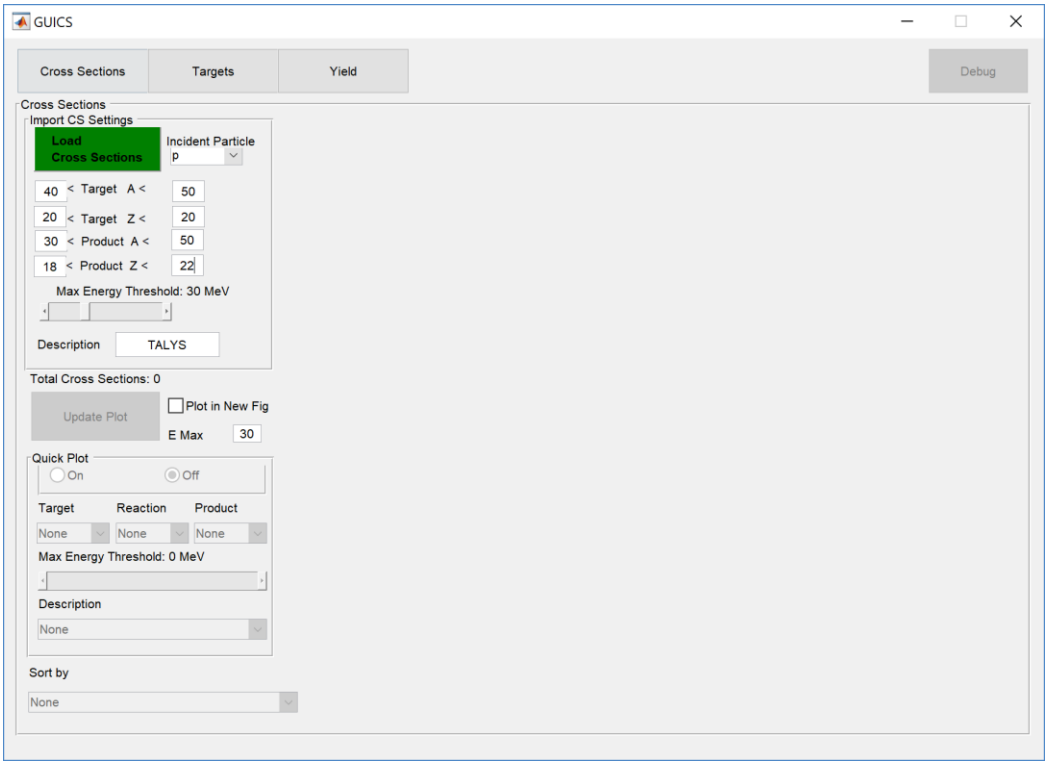
- **Note**: The application sub-folder should contain all the files found in the "for_redistribution_files_only" folder at https://github.com/dsfergus/RnPC-public-v1.1.
- **Warning**: RnPC.exe will not run if moved away from the relevant data folders; that is, the relative path from RnPC.exe to "DATA/NUDAT2-7" and the files contained within must be maintained.

RnPC Introduction – Example Use

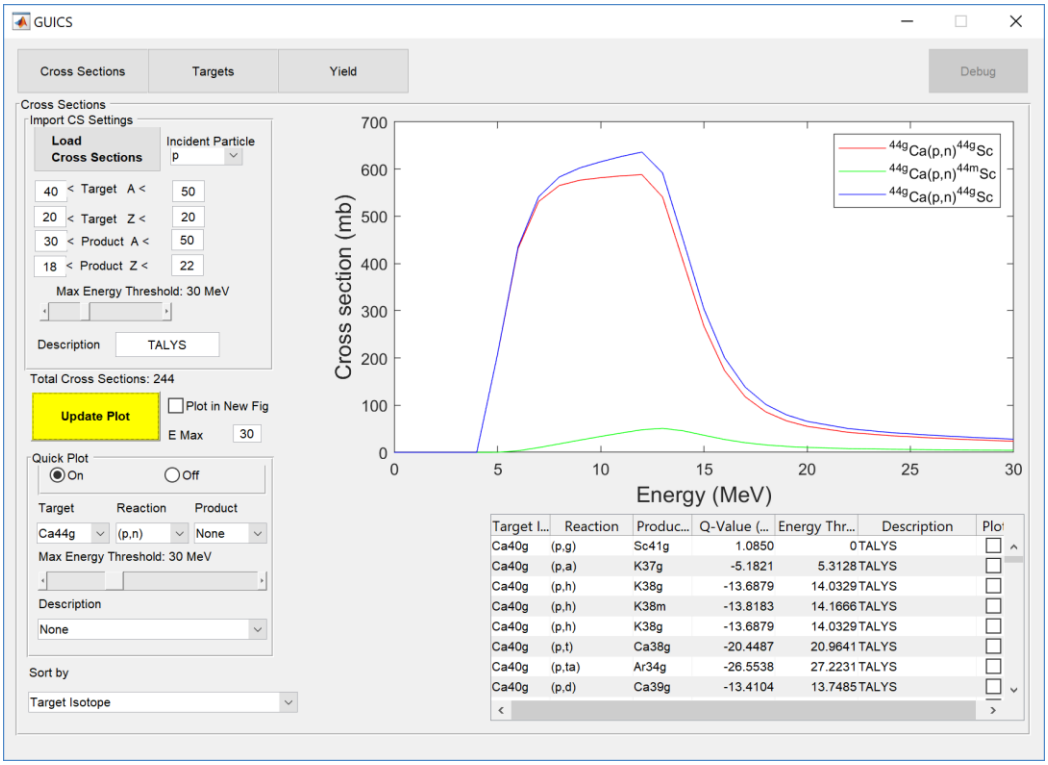
This section will introduce the user to the basic functions of the program. It can be started by executing the RnPC.exe file.

Cross Sections Tab:

The first tab is the cross sections tab. The user should load all the cross-sections required for the calculations.



- To do this, select the appropriate settings in the 'Import CS Settings' Panel.
    - For example, the settings above will only import certain cross-sections, based on if the incident particle is a proton ('p'), if the target and product isotopes have certain mass and Z numbers, and if the reaction cross section energy threshold is below 30 MeV. It will label these cross-sections as being from 'TALYS' (the default).
- Click on the green 'Load cross sections' button. This will open the window prompt. Select the folder top folder of all the cross sections. In the data provided, it is located at: $GUI_DIRECTORY$/DATA/TALYS
    - Note that this directory currently contains all the proton and deuteron induced cross-sections for Calcium and Molybdenum. If you select the top folder, it will take a while to go through all of them. You can increase the speed by selecting the cross sections of interest and putting them in a new folder.
- The cross-sections are now displayed in the table and other functions in the 'Cross Sections' tab are now available. You can plot cross section by selecting the plot checkboxes individually in the table, or by turning quickplot 'on' and using the dropdown menus and sliders. The table can be sorted by each column using the 'sort by' pulldown menu. Note that once the desired combinations of cross-sections to plot are selected, the 'update plot' button must be pressed.



Note: See Cross Section library section below for format of cross-section files and how to obtain the ones for the production calculations of interest.

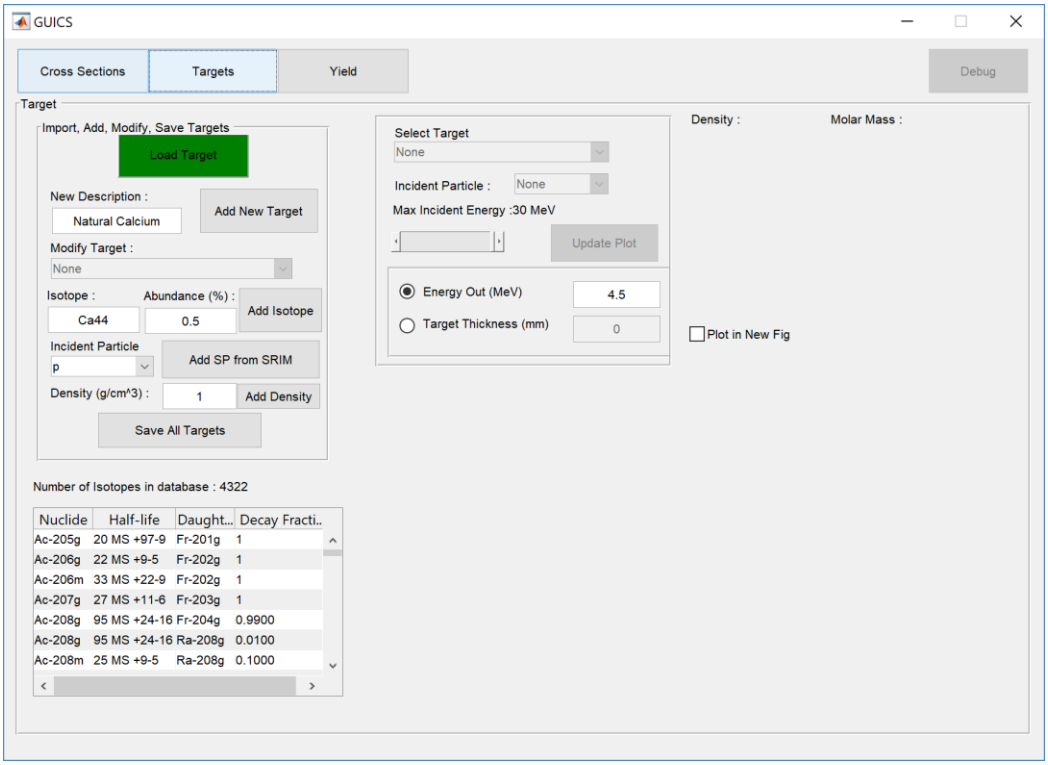
Targets Tab

The two main features of the Targets tab are the radionuclide table and the target functionalities.

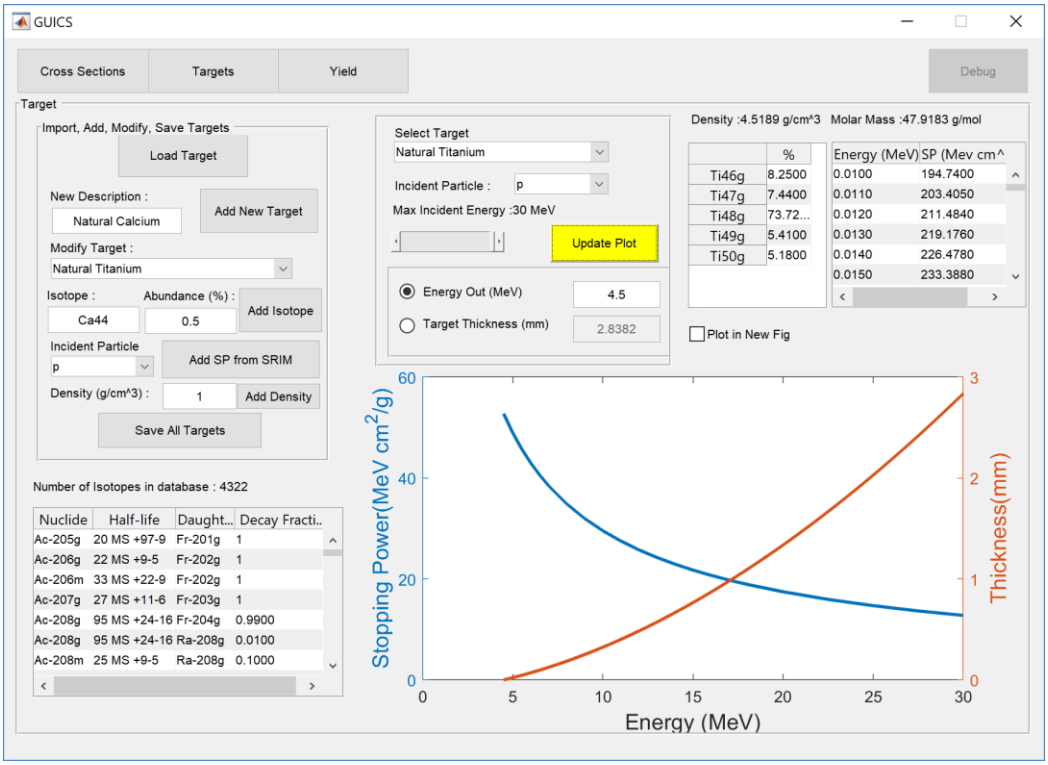
- **Note**: In order to access the main functionality of the tab, the cross-sections should have been loaded.

The radionuclide table is in the bottom right corner and displays all the nuclides in the library and their half-lives, as well as their daughter radionuclides and decay fractions if they are radioactive. See Nuclide Library below for details.

The remainder of the Targets tab can be used to load, verify and modify targets.



- The targets should be loaded next, which can be done by clicking the green ‘Load Target’ button. The user file which defines targets can be found under $GUI_DIRECTORY$/DATA and has the extension ‘.tgt’. The provided file is ‘Targets.tgt’.
- Once targets are loaded, the user can plot the stopping power and particle range for the different particles associated with the target, by clicking the yellow ‘update plot’ button. They can also look at the isotopes which are included in each target and their relative abundance.
    - For example, in the image below, the stopping power is being plotted for the protons in natural calcium, and the range is being plotted as a function of degrading the proton energy to the energy out (4.5 MeV).

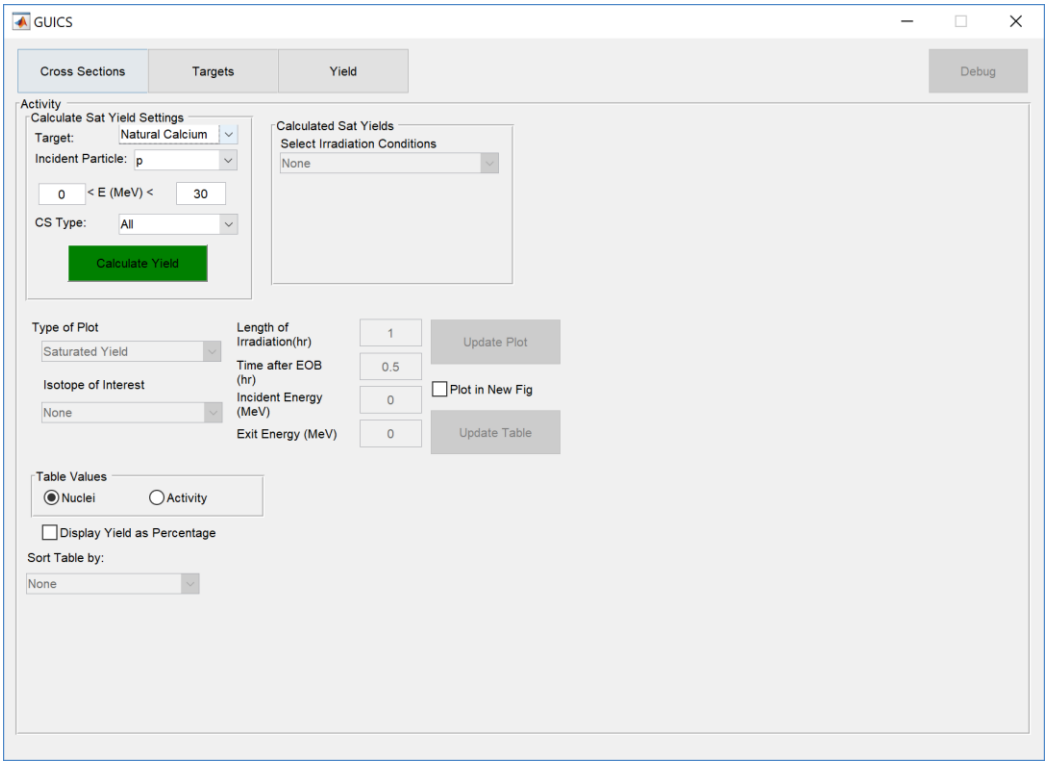


- Note: It is easier to fully define targets in a .tgt file than to specify them in the GUI. The file format can be found in the Target library section.

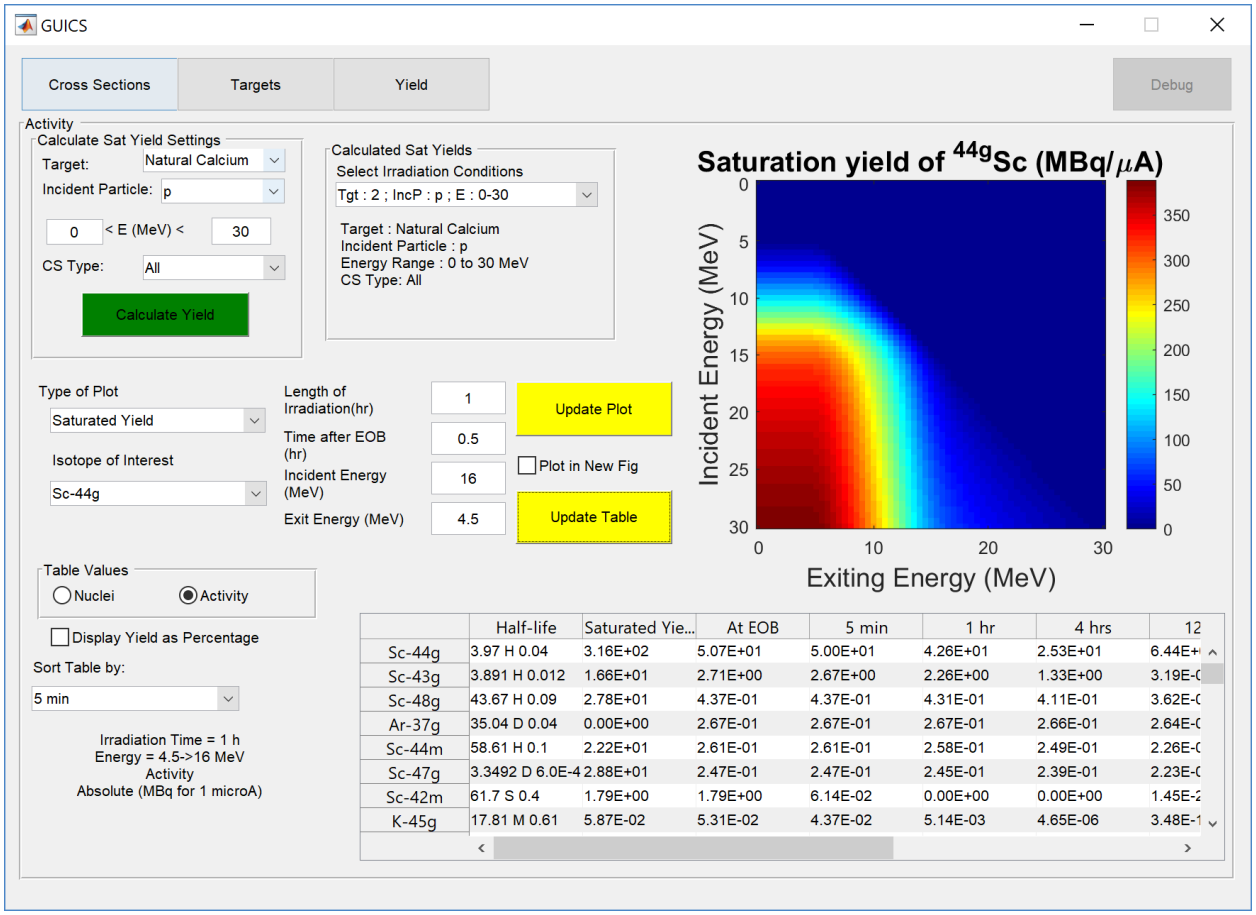
Yield Tab

The radionuclide production calculations can be performed on the Yield tab, after having loaded the cross-sections and targets.

- In the 'Calculate Sat Yield Settings' tab, select the appropriate setting and click the green 'Calculate yield' button.
    - Select the target, incident particle, and range of energies over which the saturated yields will be calculated. Also, if you only want to use a subset of the imported cross-sections, use the 'CS type' drop down menu to select the description with which they were imported. Note that using a wider energy range and a larger amount of cross-sections will increase computation times.
    - **Note**: If there are no cross-sections for any of the nuclides in the target selected for the incident particle selected, no yields will be calculated.



- Once the saturation yields have been calculated, it can then be selected from the 'Calculated Sat yields' panel. The user can then plot different graphs by modifying the plot settings, as well as create a table with the yields of the nuclides at different time points. You must click the yellow 'Update Plot' and 'Update Table' buttons to update each respectively.
    - **Note**: It may be useful to sort the table by EOB or 5 min to see the most abundant nuclides at EOB.



Data Details

Nuclide Library

Nuclide information for half-lives and decay chains are taken from NUDAT v 2.7.

NUDAT2_20180310_Nuclei.txt

- Data was downloaded from http://www.nndc.bnl.gov/nudat2/index.jsp
- Imported data can be verified on target tab in the table.
- The half-lives and branching ratios of radionuclides of interest should be verified for accuracy.

USER_Decay_State_Split.txt

In the downloaded NUDAT library, there is no distinguishing to which metastable state a given decay will occur. Thus, for example, all beta minus decays are determined to go to the ground state of the daughter nuclide. This file allows for the user to specify and correct the abundance of any decay mode.

Each correction must be added on its own line, according to the format below. This has been done for the decay of ^{99}Mo, in which the beta minus decay is corrected to decay to ^{99m}Tc with 87 % abundance and ^{99g}Tc with 13 % abundance.

File format

Requirement:

- Data must be tab separated

Column	Header	Example	Description
1	A	99	Atomic number of parent isotope.
2	Element	Mo	Element string of parent isotope.
3	Z	42	Proton number of parent isotope.
4	N	52	Neutron number of parent isotope.
5	MS	G	Metastable state of parent isotope
6	Dec Mode	B-	The decay mode to be split between ground state and metastable state.
7	A_D	99	The atomic number of daughter isotopes.
8	Element_D	Tc	Element string of daughter isotopes.
9	Z_D	43	Proton number of daughter isotopes.
10	N_D	56	Neutron number of daughter isotopes.
11	MS_D_1	g	Metastable state of first daughter isotope.
12	Branching_D_1	13	Branching ratio to the first daughter isotope.
13	MS_D_2	m	Metastable state of second daughter isotope.
14	Branching_D_2	87	Branching ratio to the second daughter isotope.

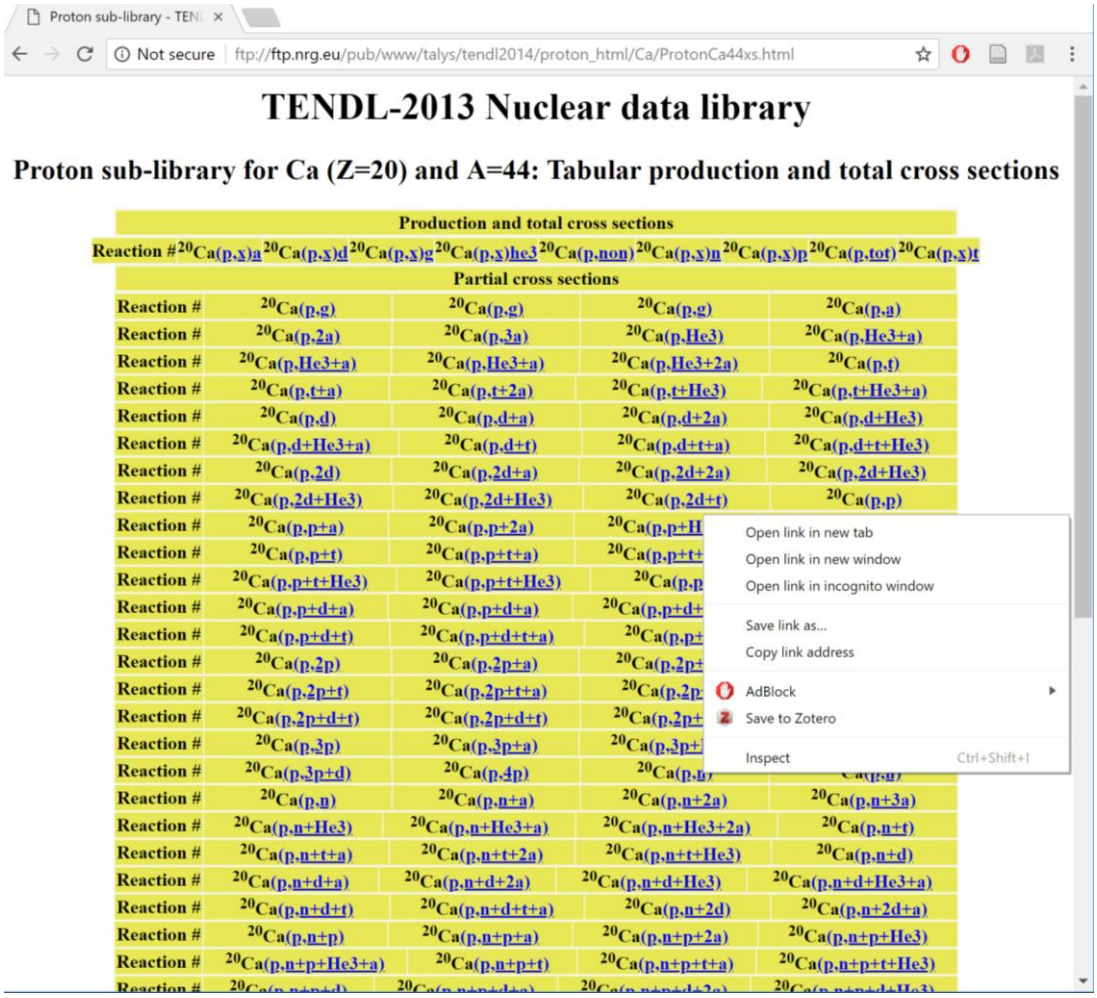
Cross Section library

The cross-sections files used in the examples are taken from TENDL-2014. This is the default file format that is used for cross-sections.

- If the same cross section is added multiple times, it may be used multiple times in the calculation of saturation yield. Ensure that the cross-section type is different for each same excitation function added in order to prevent this.
- If the partial cross-sections are added, they will take precedence over the total cross-section for that cross-section type.
    - Ex. Total cross section ^{44g}Ca(p,n)^{44}Sc is added, as well as the ^{44g}Ca(p,n)^{44g}Sc and the ^{44g}Ca(p,n)^{44m}Sc are added with the same CS type (description).
        - Yields for ^{44g}Sc and ^{44m}Sc are computed from ^{44g}Ca(p,n)^{44g}Sc and ^{44g}Ca(p,n)^{44m}Sc, ^{44g}Ca(p,n)^{44}Sc is ignored

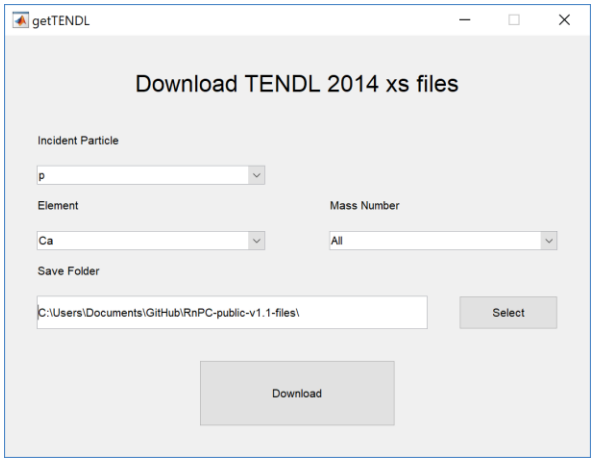
Downloading TENDL files

The TENDL-2014 files can be obtained by visiting ftp://ftp.nrg.eu/pub/www/talys/tendl2014/tendl2014.html. For example, the ^{44g}Ca(p,n)^{44g}Sc file can be obtained at: ftp://ftp.nrg.eu/pub/www/talys/tendl2014/proton_html/Ca/ProtonCa44xs.html and saved by right clicking and selecting “Save link as”.



Downloading multiple TENDL files

The getTENDL.exe file can be used to download multiple TENDL2014 files automatically. It uses ftp commands to navigate the file structure and download the cross-sections for the selected incident particle and element. It can either download the files for all mass numbers or for the specified number. The user should be careful to select only the files of interest as having a larger number of files will slow down the application.



These will download all the files for proton

User specified cross-sections

The user can also add any cross-section data they wish from any source. However, the TENDL-2014 format is the one that can be parsed and added to the database. For this reason, there are a few requirements:

- Extension must be named xs** to be imported
- Must be formatted the same as TENDL-2014. If adding experimental cross-sections, it is easiest to download the corresponding TENDL file and keep the header information. The data from or similar source can be copied, with energy in first column and cross-section (in mb) in second column

File format

For total cross-sections (that aren't split between ground and metastable states) vs. for level (matched with nuclide by energy level.

```
# p +  44Ca    : (p,n)              Total
# Q-value     =-4.43503E+00
# E-threshold= 4.60609E+00
# # energies =  45
#     E           xs        gamma xs  xs/res.prod.xs
 1.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 2.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 3.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 4.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 5.00000E+00 2.06212E+02 1.68797E+02 1.00000E+00
 6.00000E+00 4.34936E+02 5.64220E+02 9.99994E-01
 7.00000E+00 5.41498E+02 8.70923E+02 9.99978E-01
 8.00000E+00 5.83299E+02 1.09074E+03 9.99950E-01
 9.00000E+00 6.02596E+02 1.26017E+03 9.99912E-01
 1.00000E+01 6.15443E+02 1.40426E+03 9.99870E-01
```

```
# p +  44Ca    : (p,n)              Level  0
# Q-value     =-4.43503E+00 Elevel=   0.000000
# E-threshold= 4.60609E+00
# # energies =  45
#     E           xs        Branching
 1.00000E+00 0.00000E+00 0.00000E+00
 2.00000E+00 0.00000E+00 0.00000E+00
 3.00000E+00 0.00000E+00 0.00000E+00
 4.00000E+00 0.00000E+00 0.00000E+00
 5.00000E+00 2.06037E+02 9.99153E-01
 6.00000E+00 4.31610E+02 9.92352E-01
 7.00000E+00 5.31299E+02 9.81165E-01
 8.00000E+00 5.65244E+02 9.69047E-01
 9.00000E+00 5.76538E+02 9.56758E-01
 1.00000E+01 5.81668E+02 9.45120E-01
```

Target library

The target file can be used to specify the nuclides present in the target material. The abundance of the nuclides is in terms of their relative abundance in the target material. The stopping power to be used in the calculations for each different incident particle can be specified using the "# SRIM" tag.

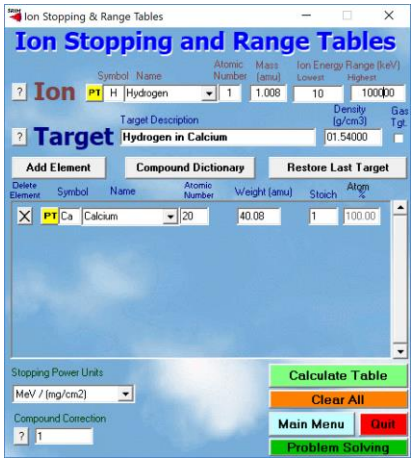
Target file formatting

TGT File format

```
# STARTTGT
# DESCRIPTION
Natural Titanium
# DENSITY
4.5189
# ISOTOPES
Ti46g 0.0825
Ti47g 0.0744
Ti48g 0.7372
Ti49g 0.0541
Ti50g 0.0518
# SRIM
pd
SRIM/HydrogeninTitanium.txt
ah
SRIM/HeliuminTitanium.txt
# STARTTGT
# DESCRIPTION
Natural Calcium
# DENSITY
1.54
# ISOTOPES
Ca40g 0.96941
Ca42g 0.00641
Ca43g 0.00135
Ca44g 0.02086
Ca46g 4e-05
Ca48g 0.00187
# SRIM
pd
SRIM/HydrogeninCalcium.txt
ah
SRIM/HeliuminCalcium.txt
#ENDFILE
```

Using SRIM for stopping power

The user has the option to manually input the stopping power or use the SRIM files. This method is recommended. SRIM can be downloaded here: http://www.srim.org/SRIM/SRIMLEGL.htm



- It is recommended to output stopping power up to 100 MeV
- **Note**: Density and stopping power required for calculation of target thickness
- If SRIM file is specified, density is updated by value in SRIM file. This can be overwritten by defining the "# DENSITY" tag underneath the "# SRIM" tag.

SRIM File format

```
 ==================================================================
              SRIM version ---> SRIM-2013.00
              Calc. date   ---> January 28, 2016
 ==================================================================

Disk File Name = SRIM Outputs\Hydrogen in Calcium.txt

Ion = Hydrogen [1] , Mass = 1.008 amu

Target Density =  1.5400E+00 g/cm3 = 2.3138E+22 atoms/cm3
======= Target  Composition ========
   Atom   Atom   Atomic    Mass
   Name   Numb   Percent   Percent
   ----   ----   -------   -------
    Ca     20    100.00    100.00
====================================
Bragg Correction = 0.00%
Stopping Units =  MeV / (mg/cm2)
See bottom of Table for other Stopping units

       Ion        dE/dx      dE/dx     Projected  Longitudinal   Lateral
      Energy      Elec.      Nuclear     Range     Straggling   Straggling
 -------------  ---------- ---------- ----------  ----------  ----------
 10.00 keV   2.594E-01  3.530E-03    2217 A      1022 A       919 A
 11.00 keV   2.706E-01  3.358E-03    2403 A      1062 A       965 A
 12.00 keV   2.811E-01  3.204E-03    2586 A      1099 A      1009 A
 13.00 keV   2.911E-01  3.066E-03    2765 A      1133 A      1050 A
 14.00 keV   3.005E-01  2.941E-03    2940 A      1164 A      1089 A
 15.00 keV   3.095E-01  2.827E-03    3112 A      1194 A      1126 A
 16.00 keV   3.180E-01  2.723E-03    3282 A      1222 A      1162 A
 17.00 keV   3.261E-01  2.628E-03    3449 A      1248 A      1195 A
 18.00 keV   3.338E-01  2.540E-03    3613 A      1272 A      1228 A
 20.00 keV   3.482E-01  2.383E-03    3935 A      1318 A      1289 A
 22.50 keV   3.645E-01  2.216E-03    4326 A      1369 A      1360 A
 25.00 keV   3.791E-01  2.074E-03    4706 A      1415 A      1424 A
 27.50 keV   3.922E-01  1.951E-03    5077 A      1456 A      1485 A
 30.00 keV   4.041E-01  1.844E-03    5440 A      1494 A      1541 A
 32.50 keV   4.147E-01  1.749E-03    5796 A      1529 A      1594 A
 35.00 keV   4.244E-01  1.665E-03    6146 A      1561 A      1645 A
 37.50 keV   4.330E-01  1.589E-03    6490 A      1591 A      1692 A
 40.00 keV   4.408E-01  1.521E-03    6830 A      1619 A      1738 A
 45.00 keV   4.541E-01  1.403E-03    7499 A      1672 A      1824 A
 50.00 keV   4.647E-01  1.304E-03    8156 A      1720 A      1904 A
 55.00 keV   4.731E-01  1.220E-03    8804 A      1764 A      1978 A
```