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A Validated MCNP(X) Cross Section Library based on JEFF 3.1

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Chapter 1

Introduction

The importance of nuclear data is often overlooked or outright ignored by many although it can make or break any calculation. One can have the best codes in the world, but if the nuclear data fed into those codes is lacking the results themselves will be worthless. Quality Assurance (QA) is therefore an important aspect in the preparation of a validated application library.
A set of library files can be considered to be a validated application library when the following requirements are met, regardless of the application or the data pre-processing codes involved in the preparation of the library [1]:

- *Verification*

  The verification process ensures that no problems were found during processing (due to faulty data, bad formatting, etc.) and that corrective actions are taken or that a warning is issued if a problem was encountered. This verification process starts even before the first library file is produced with the selection of the processing path for the data pre-processing code and all relevant parameters.

- *Validation*

  To ensure that the library is capable of providing accurate and reliable results, it must be validated. This can be done by testing the library against internationally accepted benchmarks. In order to validate nuclear data we also need to ensure that differences in benchmark results are really due to differences in data. Differences in library processing introduces "noise" and is therefore not acceptable when validating nuclear data. Examples of such influencing factors are for instance the version of NJOY (99.00, 99.90, 99.112, etc.) [2], different cross section reconstruction tolerances, etc.

- *Documentation*

  Documenting every aspect in the creation of the library is important for future reference. A data pre-processing code (in our case NJOY) should never be used as a black box. With the documentation provided with the library, a user should be capable of producing exactly the same library and understand every aspect of its creation.

Before even starting with the production of a library, it is always good to examine what has been done in the past in the field of library preparation and verification. A good place to start is the documentation of older libraries like ENDF60, ENDF66, etc.[1, 3, 4, 5] to see what NJOY processing path they had chosen, what values they used for important parameters such as the reconstruction tolerance, etc. Other important information is the type of verification tests that

were performed and what types of benchmarks were used to validate the library. And during this phase the most important question should be *why*. We should learn from all that experience and then decide upon our own approach.
All this has resulted in the creation of ALEPH-DLG (Data Library Generator) [6] and ALEPH-LIB (a multi-temperature neutron transport library for standard use by MCNP(X) [7, 8] and ALEPH [9]). ALEPH-DLG is an auxiliary computer code to ALEPH, the Monte Carlo burn-up code under development at SCK•CEN in collaboration with Ghent university. ALEPH-DLG automates the entire process of generating library files with NJOY and takes care of the first requirement of a validated application library: verify the processing. It produces tailor made NJOY input files using data from the original ENDF file (initial temperature, the fact if the nuclide is fissile or if it has unresolved resonances, etc.) When the library files have been generated, ALEPH-DLG will also process the output from NJOY by extracting all messages and warnings. If ALEPH-DLG finds anything out of the ordinary, it will either warn the user or perform corrective actions.
The temperatures included in the ALEPH-LIB library are 300, 600, 900, 1200, 1500 and 1800 K. Library files were produced for the JEF 2.2, JEFF 3.0, JEFF 3.1, JENDL 3.3 and ENDF/B-VI.8 nuclear data libraries. This will be extended with ENDF/B-VII when it becomes available. This report deals with the JEFF 3.1 files included in ALEPH-LIB that are now released by the NEA-OECD.
Another aspect that is important is maintenance and support for the library. For now, the library is limited to continuous energy neutron libraries. Proton data, data for other charged particles and $S(\alpha,\beta)$ data files will be added in the future. Questions and comments on this report and the library may be sent to Wim Haeck and Bernard Verboomen (aleph@sckcen.be). A website has also been created to keep users informed on the status of ALEPH-LIB and other related subjects (www.sckcen.be/aleph).

Chapter 2

NJOY Processing Path and Options

2.1 NJOY Version 99.112

The latest version of NJOY [2] available to us is NJOY 99.112 [10] (dated November 26, 2005). NJOY 99 is based completely upon NJOY 97 but the main goal of NJOY 99 was to incorporate cleanly a large number of changes needed for high-energy data (for instance the LA150 library [12] with data up to 150 MeV), outgoing and incident charged particles and the new photo nuclear data format of MCNP4C [13]. NJOY 2005 is currently under development at LANL but it is unclear when this new version of NJOY will become available [14].
For use under Windows and Linux, we compiled the code using the Lahey Fortran95 compiler lf95 (for both operating systems). A few minor modifications[1] were made to improve the output of the code:

- the output from the unresr and purr modules has been changed so that 6 significant digits are printed instead of 3 (unresr) or 4 (purr) because we use those numbers for QA testing.
- the variable maxscr was increased from 10000 to 50000 in the purr module to correct an error ('not enough scratch space') that occurred during the processing of ^{239}Pu of the JEF 2.2 library, this has been fixed in NJOY 99.112 but we decided to increase it to 50000 instead of 12000 (just in case).
- the line 'zero=0' was added to the reconr subroutines rdf2aa and rdf2hy to correct an lf95 compiler warning ('zero is used but never set') both in NJOY updates up92 and up99, one of them is not required.

These updates have been added to the update file up112 (used to produce the source code for NJOY version 99.112) and the file uplf95 for the Lahey Fortran95 specific updates (see appendix A). Both the file up112 and uplf95 can be found on the Los Alamos website t2.lanl.gov.

2.2 NJOY Processing and Post-Processing

NJOY is a modular program in which the different modules are called in sequence. Information is passed from module to module through the use of ENDF files. It is the NJOY module that regulates this data flow. It should be noted that data passed on in this way has all of the

[1] For NJOY 99.90 [11] we also had to make some modifications to solve memory problems and to fix compiler errors and warnings. All those things have now been fixed in NJOY 99.112.

limitations of the ENDF format. An example being the use of only 6 significant digits which can cause NJOY warnings due to round-off when passing data from one module to another (see section 3.2.1).
The NJOY processing path also depends on the type of library to be created. A continuous energy neutron library (c-type library) is created by using the following sequence of NJOY modules:

MODER 1 The first call to moder is used to convert the raw ENDF file into an NJOY binary file (binary files reduce the calculation time significantly).

RECONR The reconr module reads the data on the ENDF tape (resonance parameters and cross sections), generates point-wise energy-dependent cross sections and puts all cross sections on the same unionised energy grid.

BROADR The broadr module performs Doppler broadening to the specified temperature and thins the resulting cross section.

MODER 2 The second call to moder is used to convert the NJOY binary file into a readable ASCII file for use in ALEPH.

UNRESR The unresr module computes effective self-shielding point-wise cross section in the unresolved energy range.

HEATR 1 The first heatr run generates point wise heat production cross sections (also called kerma factors) and radiation damage cross sections.

HEATR 2 The second heatr run is used as a kinematic check to verify the correct processing in the first run.

THERMR 1 The thermr module will generate the cross sections for free scatterers in the thermal energy range.

GASPR The gaspr module will add gas production reactions to the library.

PURR The purr module will calculate the unresolved resonance probability tables used in MCNP(X).

ACER 1 This acer run will convert the previously generated data into a c-type ACE file for use in MCNP(X).

ACER 2 The second acer run reads the ACE file obtained from the previous acer run, performs the standard consistency checks and produces the final ACE file (either ASCII or binary). If problems occur, it will attempt to correct them.

Details on the input parameters for every module will follow. It is advisable to read the input specifications of the different modules of NJOY in the NJOY manuals [2, 10] before reading the part about the input parameters that we have used.
NJOY is still evolving as more features are being added (some NJOY errors and warning messages are linked to this). Until a few years ago, post-processing of the libraries was still necessary to add essential features such as delayed neutron data (which is now handled by acer as of NJOY version 99.63 [10], dated October 15, 2001), charged particle emission (handled by gaspr, an addition to NJOY 94.15, dated November 28, 1995), the addition of the probability

tables for the unresolved resonances and the gamma production data (which is now handled by acer). To prepare the standard MCNP libraries (such as ENDF60 [4] and ENDF66 [5]) LANL has had to use special post-processing codes to add some of the previous features to the final ACE tape. Post-processing is also required in the case of errors in the files. The following two problems for instance required post-processing for ENDF66:

- The heating numbers in the probability table for the unresolved energy range appeared to be inconsistent with what MCNP(X) expects. This problem has however been corrected with NJOY version 99.62 [10] (dated September 28, 2001) so it is no longer necessary to deal with this problem.
- On some platforms, it is possible that MCNP compiled in 32 bit mode will fail when it tries to read numbers smaller then $1 \cdot 10^{-37}$. To correct this problem, numbers smaller then $1 \cdot 10^{-37}$ are replaced by $1 \cdot 10^{-35}$.

As we can see, all reasons for post-processing (except for the last problem) have been dealt with in some way by NJOY. As such, we feel that our libraries will require no post-processing except maybe for the last problem if it manifests itself.

2.3 Input for MODER 1

The moder module is used to convert ENDF, PENDF (Point-wise ENDF) and GENDF (Group ENDF) files from the NJOY binary mode to formatted (i.e. ASCII) mode and vice versa. In this case, this moder run converts the raw ENDF file mounted on an ASCII tape `<raw ENDF>` (which is a positive number) to binary mode on tape `<binary ENDF>` (which is a negative number).
On older systems, the use of binary files allowed for a significant reduction in calculation time because binary files can be read faster than ASCII files. This is no longer an issue with current computer technology. The transformation of ASCII to binary is however still included because it is a good test for the formatting of an ENDF file. If there is something wrong with the formatting, this moder run will signal it.
The input instructions for this moder run would be:

```
moder
<raw ENDF> <binary ENDF>
```

2.4 Input for RECONR

The reconr module reconstructs resonance cross sections using the resonance parameters (found in file 2 in the ENDF-format) and linearises cross sections that use non-linear interpolation schemes (such as lin-log, log-lin, log-log, ...). The result is a point-wise ENDF file where all cross sections have been set on a unionised energy grid. Cross sections that are the sum of other cross sections, such as the total cross section and the total inelastic cross section, are recalculated as the sum of their constituent cross sections. All the cross sections are reconstructed to within a user specified accuracy. This module is always the first to be run because other modules, such as broadr, require linearised cross sections and/or an unionised grid.

The input instructions for reconr consist of 5 lines. The first line is used to specify the binary input tape <binary ENDF> and the binary output tape <binary out>, only two tapes are required (other modules will require more input and output tapes). The second line contains the new label <label> (delimited by single quotes) for the ENDF tape (the first line of the ENDF file). The third line specifies the ENDF material number <mat> along with the number of comment lines and the number of user defined energy grid points (both of these have been set to 0 as we do not require these features).
The fourth line is the most important line as it controls the accuracy of the reconstruction. It is used to set the following variables:

- <err>: the fractional reconstruction tolerance used when the resonance integral criterion (<errint>) is not satisfied
- <tempr>: the reconstruction temperature (which is normally 0.0 K, but there exist ENDF-files that use 77.0 K as initial temperature)
- <errmax>: the fractional reconstruction tolerance used when the resonance integral criterion (<errint>) is satisfied (the default is 10*<err>)
- <errint>: the maximum allowed resonance integral error specified in barns (the default is <err>/20000)

The linearisation process works as follows. First, the cross section is linearised until the cross section at the midpoint between two grid points is within a fraction <errmax> from the real cross section. If the contribution of this interval to the error on the resonance integral (with a $1/E$ weight):

$$\int \frac{\sigma(E)}{E} dE \tag{2.4.1}$$

is smaller than the maximum resonance integral error <errint>, than the cross section is declared converged. If the resonance integral criterion is not satisfied, <err> is used (a reasonable value would be 0.001). This is done to control the size of the file because a lot of cross section points are added due to resonances. To achieve maximum accuracy, we set <errint> to a small number (for instance 1e-12)) and <errmax> equal to <err> so that the entire cross section is linearised using <err>.
To generate the standard MCNP library ENDF66 [1, 5], LANL simply used the default values for <errmax> and <errint>, as a compromise between accuracy and library size. To use the defaults, we only need to replace the fourth line with the following line:

```
<err> /
```

The fifth line is used to terminate the input for the reconr module (if there were comment lines or user specified points, they would be inserted into the input instructions before this last line). The input instructions for reconr now are:

```
reconr
<binary ENDF> <binary out>
<label>
<mat> 0 0
<err> <tempr> <err> 1.e-12
0 /
```

2.5 Input for BROADR

The broadr module is used to generate Doppler-broadened cross sections using a point-wise ENDF-file. The basis for the reconr module is the SIGMA1 code (version 77-1, dated 1977), which is still part of the PREPRO codes [15] (under an evolved form). To verify the correctness of the cross sections generated by NJOY, we can use PREPRO to Doppler-broaden the same cross section and compare them.
The input instructions for broadr are quite similar to those of reconr. The first line specifies the input tapes (the binary ENDF tape `<binary ENDF>` and the output tape from reconr `<binary in>`) and the output file `<binary out>` for use in the following NJOY module.
The second line is used to specify the ENDF material number `<mat>` of the material that needs to be broadened. The following number is used to set the number of temperatures to which we want to broaden the cross sections. Because we will only broaden to a single temperature at a time, this has been set to `1`. The following numbers are only important when multiple temperatures are used so they have been set to `0`. The last and final entry on this line is the temperature from which the broadening will start, this is the same temperature `<tempb>` that we used in the reconr module.
The following line is practically the same as the fourth line of reconr to specify the accuracy of the broadening. The only difference is that the second entry is the maximum energy above which no broadening will be performed. This value is set to `1e+6` eV by default. To be consistent with reconr, all the other entries on this line are the same as the entries of reconr.
As was the case with reconr, LANL simply used the default values to generate ENDF66 as a compromise between accuracy and library size. To use the defaults, we only need to replace the third line with the following line:

```
<err> /
```

The fourth line specifies the temperature `<tempb>` to which we will broaden. The input instructions for broadr are terminated after this line.
The input instructions for broadr now are:

```
broadr
<binary ENDF> <binary in> <binary out>
<mat> 1 0 0 <tempr>
<err> 1e+6 <err> 1.e-12
<tempb>
0 /
```

2.6 Input for MODER 2

This moder run converts the binary tape `<binary in>` (which is a negative number) to ASCII mode on tape `<ALEPH tape>` (which is a positive number). This last tape can now be used for further verification such as plotting, ... The input instructions for this moder run would be:

```
moder
<binary in> <ALEPH tape>
```

2.7 Input for UNRESR

The unresr module produces self-shielded cross sections in the unresolved resonance range. For our purposes it is not necessary to run this module because the purr module will deal with the unresolved resonance range using probability tables. However, as part of the QA of the library, some results from unresr are compared to purr (see section 3.2.3). This module will only be run if there are unresolved resonances present in file 2 of the ENDF file.
As usual, the first input line specifies the input files (the binary ENDF tape `<binary ENDF>` and the output tape from broadr `<binary in>`) and the output file `<binary out>` for use in the next NJOY module.
The next line is used to specify the material material number `<mat>` along with the number of temperatures (set to `1` as we only calculate one temperature at a time) and the number of σ_0 values used in the calculation (which has been set to `9`, see below on why we choose 9 σ_0 values). The last number on this line is the print option. As we will require some of the output of unresr to verify the purr output, we set this option to `1` (maximum output).
The third line is used to specify the temperature `<tempb>` at which the cross sections are to be calculated. This temperature is the temperature to which the cross sections have been broadened.
The fourth line is used to specify the σ_0 values. σ_0 represents the effects of all other isotopes in the mixture on the self-shielding effect of the flux. The value of `1e-10` is required as this represents infinity. The unresolved resonance cross sections corresponding to $\sigma_0 = 1 \cdot 10^{-10}$ are the infinite diluted cross sections. This value for σ_0 is required. For our purposes, it is not necessary to specify any more values for σ_0 as the infinite dilution cross sections are the only ones that we required [4, 5]. We decided however to add 8 more σ_0 values: `1e+8`, `1e+6`, `1e+4`, `1e+3`, `3e+2`, `1e+2`, `3e+1` and `1e+1`. These values have been chosen to reflect the values used by LANL for the ENDF60 library with probability tables (although the documentation of this library clearly states that those multiple values of σ_0 are not required [4]). The NJOY manual [2] also states that the points `1e+3`, `3e+2` and `1e+2` are useful for ^{235}U (see page V-13 of the NJOY91 manual). The points `1e+8` and `1e+6` have been added to make the σ_0 grid more complete. The input for unresr is terminated after this line of σ_0 values.
The input instructions for unresr now are:

```
unresr
<binary ENDF> <binary in> <binary out>
<mat> 1 9 1
<tempb>
1e+10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1
0 /
```

2.8 Input for HEATR 1

The heatr module will add point-wise heating cross sections (also called kerma factors) and radiation damage energy production to the ENDF-file that we are processing. This first heatr run will add all the required reactions for acer and purr.
The input starts with the line containing the input and output files: the binary ENDF tape `<binary ENDF>`, the output tape from the previous module `<binary in>`) and the output file `<binary out>` for use in the next NJOY module.

The second line is used to specify the material `<mat>`. It is followed by the number of partial kerma's that have to be calculated next to the total kerma (mt301). We will require `4` or `5` extra kerma factors (depending on the fact if the material is fissile or not). The next number specifies the number of user *Q*-values that we wish to enter (which we set to `0`). We want to process all temperatures (although we only have one temperature in our library) so the fourth number is set to `0`. The following option is used to either transport gamma rays or to deposit their energy locally. The default for this is to transport the gamma rays (we set this to `0`). The printing option that follows has been set to `0` for minimal printing.
The third line contains the partial kerma's that we want to calculate. These partial kerma's are:

- `302`: the heat production due to elastic scattering, this is required for purr
- `318`: the heat production due to fission, this is required for purr but needs only to be added if the material is fissile
- `402`: the heat production due to (n,γ), this is required for purr
- `442`: this option is added because of a planned modification to MCNP that will allow the heating values to be for the local deposition of photon energy when users don't want to do a complete neutron-photon-heating calculation (added to NJOY version 99.85 [10], dated February 25, 2002)
- `444`: the total damage energy production

For the construction of the standard library ENDF66 [1, 5] LANL also asked for the following MTs:

- `303`: the heat production due to non-elastic reactions (all reactions but elastic scattering)
- `304`: the heat production due to inelastic scattering
- `443`: the total kinematic kerma (high limit)

As far as we know, these are not required (the final ACE final will only contain the total heating and damage energy) so we decided not to add them.
As such, the input for this first heatr run looks like (for a fissile material):

```
heatr
<binary ENDF> <binary in> <binary out>
<mat> 5 0 0 0 0
302 318 402 442 444 /
```

For a non-fissile material, the `5` on line 2 is replaced by `4` and the kerma `318` is removed from the last line.

2.9 Input for HEATR 2

This second heatr run is simply to check if everything is processed correctly. This type of run is also referred to as the kinematic check (see the NJOY91 manual [2] page VI-18). The input for this heatr run is quite similar to that of the previous heatr run. The only difference is that the printing option is set to 2 (maximum output with checking) and that we now ask for 6 partial kerma's for fissile material or 5 for a non-fissile material. The only extra kerma added is 303. The output of this heatr run is not used for anything and so we write it to a temporary tape <binary scratch>. The input for this heatr run will be (for a fissile material):

```
heatr
<binary ENDF> <binary in> <binary scratch>
<mat> 6 0 0 0 2
302 303 318 402 442 444 /
```

For a non-fissile material, the 6 on line 2 is replaced by 5 and the kerma 318 is removed from the last line.

2.10 Input for THERMR 1

The thermr module generates point wise neutron scattering cross sections in the thermal energy range and adds them to the library. As was the case for the unresr module, it is not required to run this module to create an MCNP(X) library [4]. For the creation of the ENDF66 libraries, thermr wasn't even used [5, 1]. We include it here for completeness.
As usual, the input begins with the input and output files. The binary ENDF tape <binary ENDF> and the output tape from the first heatr run <binary in>) are read in and the new file is written to the output file <binary out> for use in the next NJOY module.
The second input line specifies the material to be read from the ENDF input tape <binary ENDF> (which we set to 0) and the material <mat> to be read from the input tape <binary in>. Next we have to select the number of equi-probable angles (which we set to 16). The next option is 1 as we only calculate one temperature. The next two options are used to specify the inelastic and elastic option (iinc and icoh). We choose the free gas (iinc = 1) as inelastic option and no option for the elastic option (icoh = 0). We only have one principal atom so the next number is 1. The inelastic reaction will be written to mt number 221 (the special mt number for free gas). For the output option we choose maximum output with intermediate results (option 2).
The third line is used to specify the temperature <tempb> and the fourth line is used to set the tolerance (which we set to the tolerance <err> used in broadr and reconr) and the maximum energy for thermal treatment (we choose 5 eV).
The input for this module will therefore be:

```
thermr
<binary ENDF> <binary in> <binary out>
0 <mat> 16 1 1 0 1 221 2
<tempb>
<err> 5
```

2.11 Input for GASPR

The gaspr module adds charged particle production (also called gas production). The module takes any cross sections of reactions in which secondary particles such as protons, α-particles, ... are produced and adds the particle production from those cross sections to the library.
The input for this module is quite simple, just the standard line of input and output files: the binary ENDF tape `<binary ENDF>` and the output tape from the thermr module `<binary in>`) as input and `<binary out>` as output for use in the next NJOY module.
The input for gaspr will therefore be:

```
gaspr
<binary ENDF> <binary in> <binary out>
```

2.12 Input for PURR

The purr module will prepare the probability tables for the treatment of the unresolved resonance self-shielding in MCNP(X). Unresolved resonance self-shielding is already treated by the unresr module using the Bondarenko-method (also called the background cross section method). This method is however not very useful for continuous energy Monte Carlo codes. The probability table is a more natural approach to the effect of unresolved resonance self-shielding in Monte Carlo codes. When no unresolved resonances are present, it is not necessary to run this module as no probability tables will be produced.
This module will construct a series of resonance ladders that obey the statistical distributions given in file 2 of the ENDF file. Each of those ladders will be sampled randomly to produce contributions to a probability table. As a convergence test, a set of Bondarenko values is calculated at the same time and another set is calculated using the completed probability table.
The input for purr is quite similar to that of the unresr module (as both modules serve the same purpose). Again, the first line are the input (the binary ENDF tape `<binary ENDF>` and the output tape from the gaspr module `<binary in>`) and output files (`<binary out>`).
The second line has the same numbers as the second line from unresr: the material `<mat>`, the number of temperatures (`1`) and the number of σ_0 values (`9`). The following two values are the number of probability bins and the number of resonance ladders that will be used to calculate the probability table. We have set the number of probability bins to `20`, as is the case for the standard ENDF60 [4] and ENDF66 [1, 5] libraries. For most practical applications, it is accepted that a table with 10 bins will be sufficient [16], so our choice of 20 bins is acceptable. For the construction of ENDF60 and ENDF66 libraries, LANL used 32 resonance ladders but apparently this was not enough for certain isotopes (such as ^{235}U, ^{236}U and ^{239}Pu). The number of resonance ladders was raised to 64 for those isotopes. Tests have also shown that the probability tables change according to the number of resonance ladders used. We have therefore chosen to use `64` resonance ladders by default for every isotope. The following number is the printing option which we set to `1` (maximum output, we will need the result for the QA of the library). The last number allows us to set the number of energy points desired. This has been set to the default value (`0`, calculate all points).
The third and fourth line are the same as the lines for unresr: the temperature `<thermb>` and the σ_0 values. The purr input is therefore:

```
purr
<binary ENDF> <binary in> <binary out>
```

```
<mat> 1 9 20 64 1 0
<tempb>
1e+10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1
```

2.13 Input for ACER 1

The acer module prepares libraries in the ACE format (A Compact Endf) for the MCNP(X) continuous-energy Monte Carlo code. The ACE format contains all the details of the normal ENDF format but the representation of the data is different for the sake of efficiency. All cross sections share a unionised energy grid. Cross section for reactions that are the sum of others (such as the total cross section or the total inelastic cross section) are removed and will not be added to the library (they will be reconstructed when necessary by MCNP(X)). Angular distributions are converted into 32 equi-probability bins or cumulative probability distributions. Detailed photon data will be generated directly from files 12, 13, 14, 15 and 16 if they were present in the ENDF file. Charged particle production cross sections are also added to the ACE file.
This first acer run will convert the previously calculated point-wise ENDF file along with other data from the original ENDF file into an ACE file. The second acer run will perform consistency checks of this ACE file and correct the problems if possible.
The first line of the acer input specifies the input and output files. There are normally three input files. The first is the original ENDF file `<binary ENDF>`. The second file is the point-wise ENDF file `<binary in>` from the gaspr or purr run. The third input file was normally used to input the 30-by-20 photon production matrix. This has now become obsolete as the photon data is read directly from the original ENDF file (if the option `<iopp>` on line 5 is set to `1`, which is the default value). This input tape has therefore been set to `0`. After these three input files, we need to specify two output files: the new ACE file `<ACE tape>` and a file for the new xsdir entry. The ACE file will however be checked by the second acer run and the xsdir entry for the library will be generated by that run. The fifth entry on the first line is therefore set to `<scratch>`, a temporary file.
The second input line sets the basic characteristics of the library. The first number (often referred to as `iopt`) sets the type of library. We want a fast data library so `iopt` is set to `1`. The second entry determines the output from the module. No output is required from this run (comprehensive output will be generated by the second run) so the following number is `0`. The following two numbers are the ACE file type `<ntype>` (which we have set to `1` for ASCII tapes) and the library suffix `<suff>` (specified by the user). Because we do not want to read any extra pairs of `iz` and `aw`, the last number on this line is `0`.
The third line is simply a label `<label>` for the library. The fourth line sets the material `<mat>` and the temperature `<tempb>` of the library. The fifth line is used to add certain options to the ACE file. The first is the use of the new format for MCNP4C-type libraries and the second is whether or not to include detailed photon data (the `<iopp>` option mentioned earlier). Both are `1` by default. The last input line is used to specify if we want to thin the cross sections (using the defaults will not thin any cross section, which we will use). The input for this acer run will be:

```
acer
<binary ENDF> <binary in> 0 <ACE tape> <binary scratch>
1 0 1 <suff> 0
<label>
```

```
<mat> <tempb>
1 1
\
```

2.14 Input for ACER 2

As mentioned before, this acer run will perform a number of consistency tests on the produced ACE file and try to correct any problems that might surface. This run will also produce the ACE file in the format requested by the user (either an ASCII file of binary file). Please note that binary files generated by NJOY can only be used on the system on which they were created. The input for this acer run is quite similar to that of the previous run.
The first input file has been set to `0` as we will not be needing it. The second input file is the ACE file `<ACE tape>` produced in the previous run. When performing ACE consistency runs, the third entry on this line is not used for an input file but for an output file `<plot file>` (a positive number because it is an ASCII file) containing plot instructions for viewr and/or plotr. The last two files will be the final ACE file `<final ACE>` and the file `<xsdir>` containing the xsdir line for the library.
To perform the ACE consistency check, `<iopt>` (the first entry on line 2) will be set to `7` for ASCII ACE files. The print control is set to maximum (`1`). The type `<ntype>` of ACE file is either `1` for an ASCII file or `2` for the binary file (specified by the user). The next number is `-1` to specify that we do not want to change any materials in the library. This line is then followed by the label `<label>`. So the input for this acer consistency run will be:

```
acer
0 <ACE tape> <plot file> <final ACE> <xsdir>
7 1 <ntype> -1
<label>
```

Chapter 3

Library QA - Verifying Correct Processing

3.1 Introduction

When NJOY has finished creating an ACE file, the data has to be verified to ensure proper processing. Most of the time, we can rely upon NJOY itself to do this. NJOY verifies if the necessary data is available, the second acer run performs ACE consistency checks and corrects problems if any are found, ... We can however not rely on NJOY alone. So in addition to the internal NJOY processing QA, we have to perform the following steps as well:

- Check the NJOY output to analyse warning messages and errors, to verify resonance reconstruction errors, to verify the correct processing of the unresolved resonance probability table, and to process the results from the acer consistency check.
- Check cross section plots to find anomalies.
- MCNP(X) testing to see if MCNP(X) accepts the ACE file.

During the preparation of the ENDF60 [4, 3] and ENDF66 [1, 5] standard libraries, LANL also tested (and corrected) the library files using special purpose checking codes:

- CHECKTHRESH: this code performs reaction threshold processing to compare threshold energies with kinematic thresholds for negative *Q*-value reactions.
- CHECKND_NEUT: this checks the secondary neutron distributions using law 4 and 44. It verifies that the interpolation schemes are used (1 or 2), it identifies any negative probability density functions (or PDF) values and it checks if neutrons can be produced with an energy greater than the initial energy (including fission). In the case of negative PDF, the negative values are set to zero and the distribution is renormalized. It also corrects the secondary neutron distributions (except for fission) for energies greater than the incident neutron energy.
- CHECKND: this checks the secondary photon distributions using law 4 and 44.
- CHECK5: this checks data files using the mt5 reaction which is used to combine many reactions into one single reaction at high incident neutron energies (typically $\geq$ 20 MeV).
- CHECK_URES [4]: this checks the proper processing of the unresolved resonance probability tables.

None of these codes are available to us but some of them have already been added to the internal NJOY testing. All corrections and tests of CHECKTHRESH are now performed by default by the reconr module, see section 3.2.1. The tasks of CHECKND_NEUT and CHECKND are now performed by acer itself (see section 3.2.1) or during the acer consistency check (see section 3.2.4). Only the CHECK_URES and CHECK5 tests have not (yet) been added. Because the unresolved probability tables are a very important part of the library, we will provide testing of our own to ensure correct processing (see section 3.2.3).

3.2 NJOY Output Processing

3.2.1 Common NJOY Warnings

Whenever NJOY encounters an abnormal situation it will issue a warning message. In some cases, NJOY will take steps to correct the problem. All these messages have to be collected and understood before the produced library files can be approved. The following is a list of messages that can be encountered:

- `changed threshold from ... to ... for mt...`

  When reconr goes through the reactions given in the ENDF evaluation, it also checks the threshold energy E_{th} against the Q-value and the ratio AWR (the ratio between the atomic weight and the neutron mass) found in the ENDF file. If the condition

  $$E_{th} \geq \frac{AWR+1}{AWR}Q \tag{3.2.1}$$

  is not satisfied, the threshold energy is changed and reconr will issue this warning.

  Initially, NJOY only gave this warning if the change is greater than 0.1% but it appears that NJOY 99.90 will issue the warning regardless of the change so the majority of all warnings encountered will be this one. This warning can be ignored (or a corrected evaluation should be used). In the case of ^{9}Be and ^{31}P from JEFF 3.1, this can also lead to a warning in acer (see below) due to rounding errors.

- `---message from emerge---non positive elastic cross sections found`

  The reconr module found a non positive elastic cross section and set it a very small but positive value. In older evaluations, the negative cross section is most likely caused by the use of Single Level Breit Wigner (SLBW) to represent the resonance parameters in file 2. Although the use of SLBW is now discouraged in favour of formalisms such as Multi-Level Bright Wigner (MLBW), R-matrix, Reich-Moore and R-function formalisms, it is still possible to have negative scattering cross sections (see [17], p 2.34 to 2.36). In JEFF 3.1, the following nuclides are known to have this problem: ^{40}Ar, ^{61}Ni, ^{111}Cd, ^{113}Cd, ^{128}Te, ^{157}Gd, ^{182}W and ^{244}Cm.

- `---message from lunion---xsec nonzero at threshold for mt=...`

  The initial value of a threshold reaction cross section is different from zero. NJOY has corrected this by using a jump in the cross section at the threshold energy. Because of this correction, acer and MCNP(X) will however give a warning concerning coincident energy points (see below). This message can be ignored, but the evaluation should maybe be corrected as well. The following nuclides in JEFF 3.1 are known to have such cross section jumps: ^{16}O, ^{19}F, ^{23}Na, ^{35}Cl, ^{37}Cl, ^{150}Nd, ^{155}Eu, ^{204}Pb and ^{243}Am.

- `---message from hinit---mf4 and 6 missing, isotropy assumed for mt...`

  The ENDF file contains cross sections in the mt600 to mt800 range but these do not have corresponding entries in file 4 (angular distributions) or file 6 (energy-angle distributions). In order to continue, NJOY assumes an isotropic angular distribution. This message can be ignored, but the evaluation should maybe be corrected as well.

- `---message from hinit---mt18 is redundant`

  In the ENDF format, mt18 (total fission) is always the sum of mt19, mt20, mt21 and mt38. If any of these are present, heatr will use the spectra associated with these mt-numbers and ignore the spectrum of mt18. This is just an informative message and can be ignored.

- `---message from hinit---mt19 has no spectrum`

  As mentioned before, mt18 (total fission) is the sum of mt19, mt20, mt21 and mt38. In some evaluations, these partial fission reactions are given but they have no spectrum associated with them. heatr will now assume that the spectrum associated with mt18 has to be used instead. This is just an informative message and can be ignored.

- `---message from hinit---mt458 is missing for this mat`

  Energy release in fission for incident neutrons (mt458) is missing from the ENDF file of a fissile nuclide. No partial components of the fission energy release are given while they are required to calculate the heating. This message can be ignored, the only solution is to use a corrected evaluation which includes mt458.

- `---message from hinit---mf6, mt... does not give recoil za=...`

  The energy-angle distribution for the specified particle is missing in file 6. NJOY requires energy distributions for all secondary particles from a reaction to compute the energy deposition. In this case, NJOY has to make an assumption and generate an approximate to the data needed. This message can be ignored, but the evaluation should maybe be corrected as well.

- `---message from nheat---changed q from ... to ...`

  NJOY does not include energy from delayed emission (gammas and betas) in the prompt heating. The fission Q-value is changed from the total value given in file 3 to a prompt value using the delayed neutron energy from mf1, mt458. This is just an informative message and can be ignored.

- `---message from sixbar---no distribution for mt... particle ...`

  The ENDF6 format allows an evaluator to describe a subsection of file 6 using LAW=0 (no distribution given). This is fine for particle yields for gas production, ... but they are not adequate for computing heating and damage. This can be ignored if no corrected evaluation is available. In JEFF 3.1 this message is issued for mt5 in the following evaluations: all Ca isotopes, ^{45}Sc, all Fe isotopes, all Ge isotopes, ^{99}Tc, all Pb isotopes and ^{209}Bi. The mt5 reaction number is a lump reaction number for neutron energies above 20 MeV so for normal applications this should not pose a problem.

- `---message from h6ddx---vertical segment(s) in distribution y(x) is ill defined`

  This error is issued for ^{56}Fe.

- `---message from ptleg2---negative probs found`

  Secondary particle energy and/or angle distributions can be represented using a infinite serial decomposition in Legendre polynomials. Because an infinite series is not practical, it has to be cut off at a certain order (in the ENDF format, the upper limit is 64). Because the Legendre polynomials are not necessarily positive, this can introduces areas where the series leads to negative values - which is physically impossible. An evaluation with this error should be corrected (for instance by using a higher order cut-off).

  This message occurs when the acer module has found such a negative probability distribution function (or PDF) value. To "solve" the problem, acer has set the value to zero and has renormalized the distribution back to 1. The CHECKTHRESH code was used to verify and correct this in the case of ENDF60 and ENDF66 (before it was added to NJOY). Table 3.1 gives an overview of all evaluations in JEFF 3.1 with this error.

- `---message from ptleg---negative area between mu=... and ..., ...,  e= ...`

  The ptleg subroutine of the acer module translates ENDF Legendre angular distributions into tabulated form with equal probability μ intervals. In this routine the cosine interval μ = -1 to 1 is divided into 1000 intervals and integrated. When the integral of the angular distribution over such an interval is negative, we receive this message. This is caused by the fact that the Legendre polynomial series can lead to negative values (see the ptleg2 problem on negative probabilities). ^{16}O from ENDF/B-VI.8 (which has been taken over to JEFF 3.1) is known to have this problem.

- `---message from unionx---threshold error`

  This error is encountered for instance for ^{9}Be and ^{31}P from JEFF 3.1. This error normally surfaces when there is an inconsistency between the threshold energy of a reaction in the ENDF file and the value calculated by NJOY (see the first error described in this section). This is already checked and corrected in reconr so this error should never occur. However, NJOY uses ENDF files to transfer information between modules in which any number is rounded to 6 significant digits. In the case of the above mentioned nuclides, the difference between the calculated value and the one in the ENDF file occurs in the 7th significant digit (which is lost due to rounding). As such, this error can be ignored. As an illustration, this is the complete message for ^{31}P:

  ```
  ---message from unionx---threshold error
                  54  3.4023020E+06  3.4023021E+06  9.9999998E-01
  ```

- `---message from consis---consistency problems found`

  The second acer run provides a consistency check of the ACE file produced by the first acer run. Whenever something abnormal is found, this message will be printed. In some cases, the error should have been corrected. See section 3.2.4 for more information.

3.2.2 Resonance Reconstruction

The reconr module reconstructs resonance cross sections using the resonance parameters and linearises cross sections that use non-linear interpolation schemes on a unionised energy grid (all cross sections of the same nuclide will use the same energy grid). During the reconstruction and linearisation of the cross section, two criteria will be used: the fractional reconstruction

Table 3.1: Overview of all nuclides from JEFF 3.1 with the ptleg2 problem: mt-numbers, energy (given in MeV) and number of negative probability values.

nuclide	mt	E	nr	nuclide	mt	E	nr	nuclide	mt	E	nr
^{10}B	2	16.5	20	^{168}Er	51	20	11	^{233}U	2	16.5	19
	2	17	15	^{170}Er	51	20	13		2	17	49
^{11}B	2	20	59	^{177}Hf	2	17	24		2	18	92
^{58}Co	2	14.5	3		2	18	17		2	18.5	122
^{101}Ru	2	6.87	20		2	19	71		2	19	18
	2	7	21		2	20	71		2	19.5	272
	2	10.5	33	^{179}Hf	2	9	66		2	20	272
	2	11	90		2	14	9	^{235}U	73	16	1
	2	12	171	^{197}Au	2	24	39		77	16	1
	2	13	25		2	25	96		81	16	1
	2	14	44		2	26	217	^{238}Pu	2	20	148
	2	14.5	43		2	27	228	^{244}Pu	2	15	6
	2	15	46		2	28	264		2	20	6
	2	16	77		2	29	278	^{246}Pu	2	20	89
	2	17	98		2	30	391	^{244}Am	2	19	13
	2	18	127		53	29	18		2	20	41
	2	19	164		53	30	27	^{244m}Am	2	19	13
^{106}Pd	2	14	2		56	30	9		2	20	41
	2	14.5	5	^{196}Hg	68	25	14	^{240}Cm	2	20	132
^{107}Pd	2	14.5	7	^{198}Hg	69	20	14	^{242}Cm	2	20	41
^{108}Pd	2	14.5	3	^{223}Ra	2	20	14		51	15	24
^{110}Pd	2	12	6	^{224}Ra	2	20	15		51	20	24
	2	14	5	^{225}Ra	2	20	17		52	4	8
^{109}Ag	2	15	2	^{226}Ra	2	20	17	^{243}Cm	2	20	44
	2	20	2	^{225}Ac	2	20	17	^{245}Cm	2	20	8
^{139}La	2	10	17	^{227}Ac	2	20	18	^{247}Cm	2	20	47
^{151}Sm	2	10	3	^{229}Th	2	20	20	^{248}Cm	2	20	50
^{165}Ho	2	25	67	^{230}Th	2	20	10	^{250}Bk	2	20	53
	2	30	236	^{231}Pa	2	15	2	^{254}Cf	2	20	86
	51	30	2		2	20	23	^{254}Es	2	19	31
^{166}Er	51	20	4	^{232}U	2	15	1		2	20	86
^{167}Er	51	20	9		2	20	30	^{255}Es	2	20	92
	52	20	7					^{255}Fm	2	19	30
									2	20	92

tolerance <err> and the maximum resonance integral error <errint> with its associated reconstruction tolerance <errmax>. If we asked for maximum accuracy, the tolerance <err> will be used in the linearisation of the entire cross section. As a result, the file will be rather large due to the large number of points. To avoid large files, the maximum resonance integral error <errint> and the reconstruction tolerance <errmax> are used. In that case, the tolerance <errmax> will be used for the linearisation of the cross section if the error on the resonance integral satisfies the maximum resonance integral error <errint>. If this is not the case, the cross section is linearised to within <err>.
After finishing the reconstruction, the reconr module will print a summary table of the possible resonance integral error due reconstruction process. This table must be checked to see if the error is not too large. For ^{238}U from JEF 3.1 (using <err> = 0.001 and the default values for the other tolerances), this summary looks like this (some lines were cut to save space):

```
             estimated maximum error due to
             resonance integral check (errmax,errint)

  upper      elastic   percent   capture   percent   fission   percent
  energy     integral   error    integral   error    integral   error
1.00E-05
1.00E-04     2.17E+01   0.000    1.84E+02   0.000    1.82E-03   0.000
1.00E-03     2.17E+01   0.000    5.81E+01   0.000    5.76E-04   0.000
1.00E-02     2.17E+01   0.000    1.84E+01   0.000    1.82E-04   0.000
1.00E-01     2.17E+01   0.000    5.84E+00   0.000    5.77E-05   0.000
1.00E+00     2.16E+01   0.000    1.93E+00   0.000    1.86E-05   0.000
...
5.00E+02     1.92E+01   0.001    5.03E+00   0.014    1.89E-05   0.008
1.00E+03     1.51E+01   0.002    2.45E+00   0.045    4.10E-04   0.149
2.00E+03     1.48E+01   0.006    1.34E+00   0.129    2.91E-04   0.114
5.00E+03     1.78E+01   0.019    1.09E+00   0.362    9.05E-09   0.001
1.00E+04     1.03E+01   0.059    5.37E-01   0.912    6.96E-05   0.496
```

In the case where maximum accuracy is requested (using <err> = 0.001), the numbers in the error columns above are all zero. If the errors are too large, the user can simply decrease <err> and run NJOY again.
Just checking this table can already lead to surprising results. This is for instance the resonance reconstruction summary for elemental sulfur from ENDF/B-6.8:

```
             estimated maximum error due to
             resonance integral check (errmax,errint)

  upper      elastic   percent   capture   percent   fission   percent
  energy     integral   error    integral   error    integral   error
1.00E-05
1.00E-04     2.26E+00   0.000    3.58E+01   0.000    1.24E-01   0.000
1.00E-03     2.26E+00   0.000    1.13E+01   0.000    3.92E-02   0.000
1.00E-02     2.26E+00   0.000    3.58E+00   0.000    1.24E-02   0.000
1.00E-01     2.26E+00   0.000    1.13E+00   0.000    3.92E-03   0.000
1.00E+00     2.26E+00   0.000    3.58E-01   0.000    1.24E-03   0.000
...
5.00E+04     8.63E-01   0.006    5.22E-03   0.073    3.73E-04   1.774
1.00E+05     1.10E+00   0.003    1.53E-03   0.038    2.01E-03   1.743
2.00E+05     5.86E+00   0.001    2.04E-03   0.247    1.30E-03   1.077
5.00E+05     2.48E+00   0.010    1.22E-03   0.866    6.59E-04   1.765
1.00E+06     1.52E+00   0.018    5.29E-04   1.057    2.69E-05   2.025
```

Apparently, this element has non-zero fission integrals! This is due to the fact that the fission widths in the resonance parameters are not zero so NJOY calculates the integral. This evaluation has been in use since 1979 and was included in the beta0 version of ENDF/B-VII (in the beta1 version released in October 2005 this element was removed).
In the case of JEFF 3.1, no adjustments of the standard values of `<err>`, `<errmax>` and `<errint>` was required.

3.2.3 Unresolved Probability Tables

As was mentioned already in the introduction of this chapter, we will provide for testing of the unresolved probability tables. For this, we will perform most of the tests performed by the CHECK_URES code [4] in one form or another:

1. Compare the infinite dilution cross sections obtained from unresr by those calculated by purr and compare the infinite dilution total cross sections with the sum of the infinite dilute elastic, fission and capture cross section for both the values from unresr and purr. Fractional differences of more than $1 \cdot 10^{-10}$ are noted.

2. Compare for each probability bin the total cross section with the sum of the elastic, fission and capture cross section. Differences of greater than 1% are noted.

3. Compare the average cross section values from the ladder calculation with those obtained through the probability table itself.

4. Check if the cumulative probability is correctly normalized to 1 (give or take $1 \cdot 10^{-10}$) and check for abnormal zero probability bins.

5. Check the rows of the probability table for negative sections and abnormal zero cross sections.

The following is an illustration of all the tests performed in ALEPH-DLG for ^{238}U at 300 K for the energy of 20 keV. First, the infinite dilution cross sections from unresr and purr are compared. The first part of the test is the comparison of the infinite dilution values for the total, elastic, fission and capture cross sections (on the left) and the second part consists of testing whether the total value equals the sum of the three partials (on the right):

```
PURR-UNRESR infinite dilution cross section check:

                   total       elastic  ...       capture |    unresr tot      purr tot
 unresr      1.432516E+01  1.379577E+01  ...  5.293905E-01 |  1.432516E+01  1.432516E+01
 purr infd   1.432516E+01  1.379577E+01  ...  5.293905E-01 |
 purr bkgd   0.000000E+00  0.000000E+00  ...  0.000000E+00 |
 diff [%]       0.0000        0.0000     ...     0.0000    |     0.0000       0.0000
 passed?          yes           yes      ...       yes     |       yes          yes

     Passed all tests - no problems found
```

In this example, the column for the fission cross section was omitted (every value in this column was zero). When this test fails, this is mainly due to the background cross section (which is why the values of the background cross section is printed out as well).
The second stage is the comparison of the Bondarenko values obtained during the calculation of the probability table and the ones calculated using the probability table itself. Although the table contains all data for every σ_0 values that were used during the NJOY run, only the infinite dilution values are compared:

```
PURR Bondarenko values check:

    Bondarenko cross sections by direct sampling

              sigma0     p0 total      elastic ...      capture     p1 total
        1.000000E+10 1.436541E+01 1.383465E+01 ... 5.307606E-01 1.436541E+01
        1.000000E+08 1.436541E+01 1.383465E+01 ... 5.307606E-01 1.436541E+01
        1.000000E+06 1.436536E+01 1.383461E+01 ... 5.307592E-01 1.436532E+01
        1.000000E+04 1.436079E+01 1.383018E+01 ... 5.306131E-01 1.435618E+01
        1.000000E+03 1.432063E+01 1.379131E+01 ... 5.293179E-01 1.427672E+01
        3.000000E+02 1.422678E+01 1.370058E+01 ... 5.262064E-01 1.409623E+01
        1.000000E+02 1.401740E+01 1.349858E+01 ... 5.188250E-01 1.371602E+01
        3.000000E+01 1.360558E+01 1.310305E+01 ... 5.025293E-01 1.303210E+01
        1.000000E+01 1.316814E+01 1.268519E+01 ... 4.829514E-01 1.234338E+01

    Bondarenko cross sections from probability table

              sigma0     p0 total      elastic ...      capture     p1 total
        1.000000E+10 1.436541E+01 1.383465E+01 ... 5.307606E-01 1.436541E+01
        1.000000E+08 1.436541E+01 1.383465E+01 ... 5.307606E-01 1.436541E+01
        1.000000E+06 1.436537E+01 1.383461E+01 ... 5.307592E-01 1.436532E+01
        1.000000E+04 1.436095E+01 1.383034E+01 ... 5.306137E-01 1.435650E+01
        1.000000E+03 1.432210E+01 1.379278E+01 ... 5.293225E-01 1.427959E+01
        3.000000E+02 1.423104E+01 1.370482E+01 ... 5.262162E-01 1.410407E+01
        1.000000E+02 1.402651E+01 1.350768E+01 ... 5.188275E-01 1.373089E+01
        3.000000E+01 1.362018E+01 1.311771E+01 ... 5.024718E-01 1.305142E+01
        1.000000E+01 1.318591E+01 1.270308E+01 ... 4.828283E-01 1.236715E+01

    Bondarenko cross sections difference [%]

              sigma0     p0 total      elastic ...      capture     p1 total | passed?
        1.000000E+10       0.0000       0.0000 ...       0.0000       0.0000 |   yes
        1.000000E+08       0.0000       0.0000 ...       0.0000       0.0000 |
        1.000000E+06       0.0001       0.0000 ...       0.0000       0.0000 |
        1.000000E+04       0.0011       0.0012 ...       0.0001       0.0022 |
        1.000000E+03       0.0103       0.0107 ...       0.0009       0.0201 |
        3.000000E+02       0.0299       0.0309 ...       0.0019       0.0556 |
        1.000000E+02       0.0650       0.0674 ...       0.0005       0.1084 |
        3.000000E+01       0.1073       0.1118 ...       0.0114       0.1481 |
        1.000000E+01       0.1349       0.1409 ...       0.0255       0.1924 |

    Passed Bondarenko infinite dilution test
```

In the example given above, the column for the fission cross section was omitted (all values are again all zero).

The third and last stage is the testing of the probability table itself. The test again consists of two parts: an overview of the probability table (for every bin, the probability cumulative probability and the cross section values are printed) and the bin test (where the sum of the partials is compared to the total value). For our ^{238}U example the probability table overview looks like this (the bin tests were omitted due to space):

```
PURR-ACER unresolved resonance probability table check:

 bin      tot prob      cum prob         total       elastic       fission       capture
   1  4.662500E-03  4.662500E-03  3.823343E+00  3.585895E+00  0.000000E+00  2.374473E-01
   2  1.791875E-02  2.258125E-02  6.229751E+00  5.966992E+00  0.000000E+00  2.627585E-01
   3  6.367188E-02  8.625313E-02  8.460657E+00  8.200861E+00  0.000000E+00  2.597957E-01
```

```
  4  5.406562E-02  1.403187E-01  9.689484E+00  9.443480E+00  0.000000E+00  2.460040E-01
  5  5.973125E-02  2.000500E-01  1.029883E+01  1.006470E+01  0.000000E+00  2.341318E-01
  6  5.639375E-02  2.564438E-01  1.073697E+01  1.049481E+01  0.000000E+00  2.421615E-01
  7  5.767500E-02  3.141188E-01  1.108989E+01  1.082473E+01  0.000000E+00  2.651615E-01
  8  5.776563E-02  3.718844E-01  1.142084E+01  1.112118E+01  0.000000E+00  2.996622E-01
  9  5.468125E-02  4.265656E-01  1.175799E+01  1.140497E+01  0.000000E+00  3.530230E-01
 10  5.284063E-02  4.794063E-01  1.211012E+01  1.171121E+01  0.000000E+00  3.989129E-01
 11  5.945000E-02  5.388563E-01  1.251434E+01  1.205582E+01  0.000000E+00  4.585232E-01
 12  5.955312E-02  5.984094E-01  1.299979E+01  1.247663E+01  0.000000E+00  5.231506E-01
 13  6.262187E-02  6.610312E-01  1.361066E+01  1.300291E+01  0.000000E+00  6.077522E-01
 14  6.210313E-02  7.231344E-01  1.441660E+01  1.372964E+01  0.000000E+00  6.869662E-01
 15  6.502188E-02  7.881563E-01  1.554050E+01  1.475955E+01  0.000000E+00  7.809531E-01
 16  5.855312E-02  8.467094E-01  1.713908E+01  1.625956E+01  0.000000E+00  8.795226E-01
 17  6.284687E-02  9.095562E-01  1.976246E+01  1.877427E+01  0.000000E+00  9.881902E-01
 18  6.582813E-02  9.753844E-01  2.653817E+01  2.553805E+01  0.000000E+00  1.000119E+00
 19  1.940000E-02  9.947844E-01  4.153256E+01  4.053079E+01  0.000000E+00  1.001761E+00
 20  5.215625E-03  1.000000E+00  5.675590E+01  5.566543E+01  0.000000E+00  1.090471E+00

     average probability table  1.436541E+01  1.383465E+01  0.000000E+00  5.307606E-01
    average ladder calculation  1.436541E+01  1.383465E+01  0.000000E+00  5.307606E-01
                        diff [%]     0.0000        0.0000        0.0000        0.0000
                         passed?       yes           yes           yes           yes

Passed all bin tests - no problems found
Passed all average cross section tests - no problems found
Passed negative test - no negative cross section were found
Passed zero test - no abnormal zero cross section were found
```

As was indicated before, these probability table can have a number of defects. First of all, there are the possible zero cross section values. They mostly occur in the first few bins where the cross section value can become very small. This is possibly due to round-off because ENDF files are used to transfer information (the number of significant digits is limited). The following is an example for ^{144}Ce from JEFF 3.1 at 300 K (at an energy of 12.5 keV) where the elastic cross section in the first bin is zero while the elastic cross section values for bin 2 and 3 are quite low:

```
PURR-ACER unresolved resonance probability table check:

 bin      tot prob      cum prob         total       elastic       fission       capture
   1  5.918750E-03  5.918750E-03  4.427165E-04  0.000000E+00  0.000000E+00  4.427130E-04
   2  1.353125E-02  1.945000E-02  9.661759E-04  1.346222E-07  0.000000E+00  9.660378E-04
   3  5.795938E-02  7.740938E-02  7.611501E-03  1.364715E-03  0.000000E+00  6.246783E-03
   4  6.397500E-02  1.413844E-01  4.903847E-01  4.784755E-01  0.000000E+00  1.190921E-02
   5  5.536563E-02  1.967500E-01  1.183513E+00  1.170341E+00  0.000000E+00  1.317209E-02
   6  5.531875E-02  2.520688E-01  1.711335E+00  1.699135E+00  0.000000E+00  1.220037E-02
   7  5.514687E-02  3.072156E-01  2.183366E+00  2.170705E+00  0.000000E+00  1.266053E-02
   8  4.683750E-02  3.540531E-01  2.597204E+00  2.583742E+00  0.000000E+00  1.346129E-02
   9  5.892187E-02  4.129750E-01  3.046429E+00  3.029602E+00  0.000000E+00  1.682707E-02
  10  6.120000E-02  4.741750E-01  3.591510E+00  3.571395E+00  0.000000E+00  2.011522E-02
  11  6.227500E-02  5.364500E-01  4.240109E+00  4.214968E+00  0.000000E+00  2.514148E-02
  12  5.410938E-02  5.905594E-01  4.973862E+00  4.941652E+00  0.000000E+00  3.221007E-02
  13  6.009688E-02  6.506563E-01  5.898720E+00  5.852202E+00  0.000000E+00  4.651832E-02
  14  6.285625E-02  7.135125E-01  7.318426E+00  7.252548E+00  0.000000E+00  6.587885E-02
  15  6.911875E-02  7.826313E-01  9.840770E+00  9.731101E+00  0.000000E+00  1.096695E-01
  16  6.023750E-02  8.428688E-01  1.470241E+01  1.451735E+01  0.000000E+00  1.850631E-01
  17  6.598437E-02  9.088531E-01  2.714710E+01  2.687932E+01  0.000000E+00  2.677814E-01
  18  6.877500E-02  9.776281E-01  8.425859E+01  8.396091E+01  0.000000E+00  2.976748E-01
```

```
 19  1.414687E-02  9.917750E-01  1.817117E+02  1.814068E+02  0.000000E+00  3.048717E-01
 20  8.225000E-03  1.000000E+00  2.107427E+02  2.104787E+02  0.000000E+00  2.640955E-01

      average probability table  1.563706E+01  1.555737E+01  0.000000E+00  7.969520E-02
     average ladder calculation  1.563707E+01  1.555737E+01  0.000000E+00  7.969520E-02
                         diff [%]     0.0000        0.0000        0.0000        0.0000
                          passed?       yes           yes           yes           yes

 Passed all bin tests - no problems found
 Passed all average cross section tests - no problems found
 Passed negative test - no negative cross section were found
 Warning: did not pass zero test - 1 abnormal zero cross section were found
```

Negative cross section values on the other hand are physically impossible. When these occur, ALEPH-DLG will simply rerun the isotope with the unresolved probability table option switched off. For now, this is the only point where ALEPH-DLG takes corrective actions. This is an example of ^{148}Nd of JEFF 3.1 at 300 K (at an energy of 8 keV) where there are 7 negative values in the probability table (4 total and 3 capture cross section values):

```
PURR-ACER unresolved resonance probability table check:

 bin      tot prob      cum prob         total       elastic       fission       capture
   1  4.181250E-03  4.181250E-03 -4.822215E-02  1.156328E-07  0.000000E+00 -1.373847E-02
   2  1.150312E-02  1.568437E-02 -4.658385E-02  1.093039E-06  0.000000E+00 -1.210115E-02
   3  5.239688E-02  6.808125E-02 -3.997770E-02  4.144996E-05  0.000000E+00 -5.535351E-03
   4  6.160625E-02  1.296875E-01 -5.314284E-03  2.803189E-03  0.000000E+00  2.636633E-02
   5  5.971563E-02  1.894031E-01  3.755912E-01  3.083192E-01  0.000000E+00  1.017559E-01
   6  6.245937E-02  2.518625E-01  1.303667E+00  1.246896E+00  0.000000E+00  9.125447E-02
   7  6.225312E-02  3.141156E-01  2.168909E+00  2.124675E+00  0.000000E+00  7.871813E-02
   8  6.263438E-02  3.767500E-01  2.917091E+00  2.879398E+00  0.000000E+00  7.217662E-02
   9  6.926562E-02  4.460156E-01  3.638130E+00  3.614899E+00  0.000000E+00  5.771551E-02
  10  6.888437E-02  5.149000E-01  4.412159E+00  4.363108E+00  0.000000E+00  8.353441E-02
  11  6.702500E-02  5.819250E-01  5.273581E+00  5.208550E+00  0.000000E+00  9.951473E-02
  12  6.297500E-02  6.449000E-01  6.276626E+00  6.190311E+00  0.000000E+00  1.207987E-01
  13  5.291250E-02  6.978125E-01  7.435103E+00  7.309307E+00  0.000000E+00  1.602797E-01
  14  5.661875E-02  7.544312E-01  8.961360E+00  8.785904E+00  0.000000E+00  2.099398E-01
  15  5.539062E-02  8.098219E-01  1.142069E+01  1.119543E+01  0.000000E+00  2.597388E-01
  16  5.801250E-02  8.678344E-01  1.629022E+01  1.598533E+01  0.000000E+00  3.393781E-01
  17  5.465312E-02  9.224875E-01  2.924341E+01  2.881197E+01  0.000000E+00  4.659304E-01
  18  5.442500E-02  9.769125E-01  8.742029E+01  8.642198E+01  0.000000E+00  1.032795E+00
  19  1.606875E-02  9.929812E-01  2.152746E+02  2.138398E+02  0.000000E+00  1.469247E+00
  20  7.018750E-03  1.000000E-00  2.962066E+02  2.951656E+02  0.000000E+00  1.075480E+00

      average probability table  1.609580E+01  1.591664E+01  0.000000E+00  2.136386E-01
     average ladder calculation  1.609580E+01  1.591664E+01  0.000000E+00  2.136387E-01
                         diff [%]     0.0000        0.0000        0.0000        0.0000
                          passed?       yes           yes           yes           yes

 Passed all bin tests - no problems found
 Passed all average cross section tests - no problems found
 Warning: did not pass negative test - 7 negative cross section were found
 Passed zero test - no abnormal zero cross section were found
```

There is also the possibility to have bins with zero probability. In this case, the bin will never be sampled so that negative or zero cross section values in this bin do not pose a problem. This problem also surfaced during the preparation of the URES library for MCNP (the first MCNP library to include probability tables) [4] but no corrective measures where taken. It is

up to the user to decide what to do with this problem. An extreme example with 8 bins of zero probability can be found in ^{250}Cm from JEFF 3.1 at 300 K (at an energy of 150 eV):

```
PURR-ACER unresolved resonance probability table check:

 bin      tot prob      cum prob         total       elastic       fission       capture
   1  5.446875E-03  5.446875E-03  5.392441E-01  1.552841E-01  3.833252E-04  3.835767E-01
   2  1.434375E-02  1.979062E-02  1.419568E+00  8.056844E-01  6.402496E-04  6.132430E-01
   3  6.831875E-02  8.810937E-02  4.681343E+00  4.217565E+00  4.618940E-04  4.633165E-01
   4  2.525313E-02  1.133625E-01  9.316751E+00  9.032870E+00  2.973886E-04  2.835829E-01
   5  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   6  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   7  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   8  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   9  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  10  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  11  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  12  0.000000E+00  1.133625E-01  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  13  5.694969E-01  6.828594E-01  1.017317E+01  1.017317E+01  1.990072E-10  2.092492E-07
  14  6.308437E-02  7.459438E-01  1.017338E+01  1.017317E+01  2.036667E-07  2.056038E-04
  15  5.635625E-02  8.023000E-01  1.017472E+01  1.017317E+01  1.540981E-06  1.555110E-03
  16  5.392813E-02  8.562282E-01  1.018443E+01  1.017146E+01  1.247093E-05  1.295907E-02
  17  5.385313E-02  9.100813E-01  1.294963E+01  1.213710E+01  7.970381E-04  8.117332E-01
  18  6.643125E-02  9.765125E-01  3.205054E+01  2.906784E+01  2.946783E-03  2.979749E+00
  19  1.654375E-02  9.930563E-01  2.450191E+02  2.113558E+02  3.588485E-02  3.362735E+01
  20  6.943750E-03  1.000000E+00  4.276506E+03  3.836888E+03  4.816872E-01  4.391363E+02

      average probability table  4.471146E+01  4.080950E+01  4.228177E-03  3.897738E+00
     average ladder calculation  4.471146E+01  4.080950E+01  4.228177E-03  3.897738E+00
                      diff [%]     0.0000        0.0000        0.0000        0.0000
                       passed?       yes           yes           yes           yes

 Passed all bin tests - no problems found
 Passed all average cross section tests - no problems found
 Passed negative test - no negative cross section were found
 Warning: did not pass zero test - 32 abnormal zero cross section were found
 Warning: 8 zero probability values found
```

In some cases, all the problems described above can be found in a single example. This is for instance the case for the probability table of ^{22}Na from JEFF 3.1 at 300 K (at an energy of 15 keV):

```
PURR-ACER unresolved resonance probability table check:

 bin      tot prob      cum prob         total       elastic       fission       capture
   1  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   2  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   3  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   4  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   5  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   6  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   7  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   8  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
   9  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00  0.000000E+00
  10  5.852375E-01  5.852375E-01  1.056769E-01  0.000000E+00  0.000000E+00 -3.959991E-02
  11  3.289687E-02  6.181344E-01  1.056798E-01  0.000000E+00  0.000000E+00 -3.959699E-02
  12  3.425000E-02  6.523844E-01  1.056858E-01  0.000000E+00  0.000000E+00 -3.959101E-02
  13  6.732500E-02  7.197094E-01  1.057690E-01  1.138332E-08  0.000000E+00 -3.950781E-02
```

```
14  7.261250E-02  7.923219E-01  1.064582E-01  6.739630E-07  0.000000E+00 -3.881927E-02
15  5.415938E-02  8.464812E-01  1.248099E-01  1.009233E-02  0.000000E+00 -3.055926E-02
16  4.939687E-02  8.958781E-01  7.096786E-01  5.924746E-01  0.000000E+00 -2.807285E-02
17  5.180000E-02  9.476781E-01  2.888497E+00  2.760378E+00  0.000000E+00 -1.715786E-02
18  3.734063E-02  9.850187E-01  1.538414E+01  1.514680E+01  0.000000E+00  9.206328E-02
19  1.083750E-02  9.958562E-01  5.999406E+01  5.946302E+01  0.000000E+00  3.857638E-01
20  4.143750E-03  1.000000E-00  9.958044E+01  9.904143E+01  0.000000E+00  3.937373E-01

     average probability table  1.912509E+00  1.793225E+00  0.000000E+00 -2.599318E-02
    average ladder calculation  1.912509E+00  1.793225E+00  0.000000E+00 -2.599318E-02
                      diff [%]     0.0000        0.0000        0.0000        0.0000
                       passed?       yes           yes           yes           yes

Warning: did not pass 3 of 20 bin tests
Passed all average cross section tests - no problems found
Warning: did not pass negative test - 8 negative cross section were found
Warning: did not pass zero test - 30 abnormal zero cross section were found
Warning: 9 zero probability values found
```

An overview of the nuclides in JEFF 3.1 that have these problems can be found in table 3.2. Please note that nuclides that have negative values in the probability table will not have probability tables in ALEPH-LIB. Because zero probability bins and zero cross section values are not so bad, these nuclides still have probability tables in ALEPH-LIB.

Table 3.2: Overview of all nuclides from JEFF 3.1 with problems in the probability tables.

Negative cross section values			
Nuclide	T [K]	Nuclide	T [K]
^{22}Na	all	^{139}La	all
^{36}Ar	all	^{141}Pr	all
^{101}Ru	all	^{144}Nd	all
^{104}Pd	all	^{145}Nd	all
^{106}Pd	all	^{146}Nd	all
^{107}Pd	300, 600, 900, 1200	^{148}Nd	all
^{108}Pd	300, 600, 900, 1200	^{147}Pm	300, 600, 900, 1200
^{110}Pd	all	^{238}Np	300, 600, 900
^{109}Ag	300, 600, 900	^{252}Cf	300

Zero cross section values		Zero probability bins	
Nuclide	T [K]	Nuclide	T [K]
^{122}Sn	all	^{38}Ar	all
^{140}Ba	all	^{93}Zr	300, 600, 900, 1200
^{144}Ce	all	^{94}Nb	300, 600
^{180}Hf	900	^{116}Sn	300
		^{118}Sn	300
		^{124}Sn	all
		^{142}Ce	300
		^{250}Cm	all

3.2.4 ACER consistency tests

As was mentioned before, the second acer run will perform a number of consistency tests on the ACE file that was produced and to correct some of the problems that might be detected. The tests performed by acer are the following:

1. Do threshold values correspond to *Q*-values?
2. Is the energy grid monotonically increasing?
3. Check the angular distributions for the correct reference frame (either CM or LAB)
4. Check the angular distributions for unreasonable cosines
5. Is the emission energy less than the incident energy?
6. Do summation cross sections match sums?
7. Ensure that probability density functions are non-negative
8. Are only appropriate interpolation values used?
9. Do threshold reactions start with a zero cross section?

In the case of JEFF 3.1, the following consistency problems were encountered:

- `check that main energy grid is monotonic`
  `consis: energy ... less than ... (see point no. ...)`

  The energy grid constructed by reconr (and thinned by broadr) must consists of monotonically increasing energy values. The acer module has found points where this does not appear to be the case. In all cases encountered, the points in question had the same energy value (which represents a jump in the cross section) and not a decreasing energy value. This error is most likely due to rounding in the ENDF file (the ENDF format only allows for 6 significant digits). This consistency problem can therefore be ignored.

- `check reaction thresholds against q values`
  `consis: threshold ... less than the expected ... for ...`

  This is the same threshold error problem as described in one of the acer messages mentioned earlier. This consistency problem occurs for for ^{9}Be and ^{31}P from JEFF 3.1 and can be ignored. As an illustration, this is the complete message for ^{31}P:

```
consis: threshold  3.40230200E+00 less than the expected
        3.40230208E+00 for (n,n*4)
```

- `check energy distributions`

```
consis: ep.gt.epmax 8.509482E-12 with q.lt.0 for (n,x) at e
        1.000000E-11 -> 1.000000E-11
consis:   awr.lt.180---this is probably an error.
consis: shifting eprimes greater than epmax and renorming the
        distribution
```

```
check energy distributions
  consis: ep.gt.epmax 9.901826E-12 with q.lt.0 for (n,x) at e
          1.000000E-11 -> 1.000000E-06
  consis: awr.ge.180---there could be a legitimate positive-q
          channel or admixed fission.
```

This concerns a nuclide with an energy distribution where the outgoing neutron has more energy than the incoming. This is only possible for positive Q reactions (exothermic reactions) which are rare for light elements. NJOY corrects this by shifting the energies and renormalizing the distribution, but only if the atomic mass number is below 180. For nuclides with an atomic mass larger than 180, NJOY does nothing because there is a possibility to have a reaction with positive Q.

In JEFF 3.1, the first message is issued for elemental C, ^{14}N, ^{16}O, ^{27}Al, all Ca isotopes, ^{45}Sc, all Fe isotopes, ^{61}Ni, ^{62}Ni, ^{64}Ni, all Cu isotopes, all Ge isotopes, ^{93}Nb, ^{99}Tc, ^{103}Rh, ^{127}I and ^{129}Ni. The second message occurs for all Pb isotopes and ^{209}Bi.

- `check angular distributions for correct reference frame`
  `consis: should be lab: (n,n*c)`

  The reference frame used appears to be incorrect. For ENDF66, this occurred for ^{249}Cf and was corrected by simply changing the parameter in the ENDF file that sets the reference frame. For heavy nuclides this can be done but for lighter nuclides this can introduce errors. In JEFF 3.1 this problem occurs for the continuum of inelastic scattering in ^{23}Na and ^{239}Pu.

- `checking energy distributions`
  `consis: bad law44 kalbach r for (n,xd) at  1.800000E+01 ->`
  `6.609760E+00`

  This message indicates a problem in an energy distribution. For JEFF 3.1, this problem occurs only for nuclides taken over from JENDL 3.3 where file 6 mt203-207 have been defined: ^{96}Zr, ^{97}Mo, ^{100}Mo, ^{121}Sb, ^{123}Sb and all W isotopes.

  The mt-numbers mt203-207 (total production of protons, tritons, deuterons, ^{3}He and α) are redundant mt-numbers and should only be used in derived files according to ENDF format [17]. They are not used during transport in MCNP(X) because the secondary particle energy and angle distributions are associated with the reaction that creates them. This consistency problem can therefore be ignored.

- `check photon production sum`
  `consis: mismatch at  1.000001E-03  gpd=  1.040651E-01`
  `sum= 1.040869E-01`

  This error occurs for ^{95}Mo in JEFF 3.1.

Part II

A Validated Cross Section Library for MCNP(X) and ALEPH

Chapter 4

JEFF 3.1 Library Overview

4.1 Processing parameters and naming convention

ALEPH-LIB is the name of the multi-temperature library that we are providing for standard use by MCNP(X) and ALEPH. The temperatures included in this library are 300, 600, 900, 1200, 1500 and 1800 K. Library files were produced using the JEF 2.2, JEFF 3.0, JEFF 3.1, JENDL 3.3 and ENDF/B-VI.8 nuclear data evaluations. This will be extended with ENDF/B-VII when it becomes available. The distribution of ALEPH-LIB also contains all the graphs produced by NJOY during the second acer run (see section 2.14). The table of the content of the JEFF 3.1 library can be found in appendix B.

Because the library is foreseen for every-day use, certain compromises must be made between file size and accuracy. The tighter the tolerances set in NJOY, the more accurate the linearised cross sections will be to the data in the original ENDF file. Unfortunately, the more accurate the linearised cross sections are, the larger the files will be. And that will definitely have an adverse effect on calculation time (the larger the energy grid, the longer it takes to find the proper interval).

We have therefore chosen to use a cross section reconstruction tolerance of 0.1% with default values for the resonance integral checks (1% for the maximum reconstruction tolerance `<errmax>` and 5 10^{-8} for the resonance integral error `<errint>`, see sections 2.4 and 3.2.2 for more information). All nuclides that have unresolved resonances will have probability tables in the unresolved resonance energy range, except if there are occurances of negative cross section values in the table.

For the naming convention of the libraries, we choose to use `T/100` for the stable nuclides and `T/100 + 70` for the metastable nuclides (see table 4.1). For example, `95242.03c` is the library at 300 K for the ground state of ^{242}Am while `95242.79c` is the 900 K library of the metastable state of ^{242}Am.

Another method that is often suggested to identify the ground state and metastable state is to change the `ZAID` of the metastable state, for instance `95242` for the ground state and `95342` for the metastable state. We decided to use different library numbers for the ground state and metastable state instead of this method because this method has proved to be problematic with MCNPX. It leads to a fatal error in the models for proton transport, where the value of 342 is used as the atomic mass for ^{242m}Am. In other cases it did not lead to fatal errors, but the wrong value for the atomic mass was still used by MCNPX for use in the physics models.

We chose to use the same numbers for every nuclear data evaluation because there would not be enough library numbers if every nuclear data evaluation was assigned its own set of library

numbers. The user can however simply create his own xsdir file when he wishes to mix nuclear data evaluations.

Table 4.1: Library suffix numbers used for nuclides in the ground state (GS) and metastable state (MS).

T [K]	GS	MS
300	03c	73c
600	06c	76c
900	09c	79c
1200	12c	82c
1500	15c	85c
1800	18c	88c

Every nuclide is provided as a single file. This increases the potential for maintenance of the library (whenever a correction is made, the user does not have to replace huge files, just a few small ones). The file naming convention is simply `<ZAMID>_<EVAL>.<SUFF>` where `ZAMID` is the ORIGEN identification number of the nuclide, where `EVAL` is the nuclear data evaluation number (`22` for JEF 2.2, `30` for JEFF 3.0, `31` for JEFF 3.1, `33` for JENDL 3.3 and `68` for ENDF/B-VI.8) and where `SUFF` is the library suffix number (as given in table 4.1). For example, the ACE file for ^{242}Am in the ground state at 300 K from JEFF 3.1 can be found in the file `952420_31.03c` while it is `952421_31.73c` for the metastable state of the same nuclide.
The first part of the MCNP(X) xsdir file contains the atomic mass values (in units of neutron mass) used by MCNP(X) to recalculate compositions to the standard atoms barn^{-1} cm^{-1}. The standard xsdir files only contain atomic mass data for 300 to 400 nuclides. Because ALEPH requires atomic mass values for at least every nuclide possible in ORIGEN, we have decided to update those atomic mass values by using the Atomic Mass Evaluation 2003 included into NUBASE [18] from the Atomic Mass Data Center.

4.2 Known problems and fixes made to JEFF 3.1 library files

JEFF 3.1 contains a total of 381 files for neutron interaction. 380 of those files are processed without problems by NJOY. Only ^{253}Es (carried over from JEF 2.2) could not be processed, NJOY crashes on the purr module for this nuclide. This is not due to the evaluation but due to NJOY itself. This happens under Linux and Windows but there are operating systems where there are no problems [19].
It is not because NJOY produces a library file that there are no problems with the file. Take for instance ^{46}Ti. This nuclide has a negative scattering cross section at high energy, and the nuclide doesn't even have resonances (so it can't be a problem with the background cross section).
Other nuclide for which the initial library files produced errors in MCNPX runs are all Ti isotopes and ^{209}Bi. MCNPX 2.5.0 indicates cross section problems on these nuclides during runs with photon transport (this example is for ^{209}Bi):

```
error in cross-section table  83209.06c
energy in =  9.4950E-04     reaction index = 71     mt =  849001
       ty =   0     law =  4     energy out = NaN
energy in =  1.1936E-03     reaction index = 71     mt =  849001
```

```
       ty =   0     law =  4     energy out = NaN
energy in =  5.9403E-04     reaction index = 71     mt =  849001
       ty =   0     law =  4     energy out = NaN
energy in =  1.7530E-03     reaction index = 71     mt =  849001
       ty =   0     law =  4     energy out = NaN
energy in =  1.6567E-03     reaction index = 71     mt =  849001
       ty =   0     law =  4     energy out = NaN
```

The mt-number 849001 indicates the energy distribution for secondary photons from mt849 (the continuum part of the n,α reaction). The incident neutron energy given in these 5 error messages always fall between the same two points in the energy distribution: 200 eV and 2000 eV:

```
 0.000000+0 2.000000+2         14          0         32         168325 684931578
 8.521680+5 5.459981-3 7.323380+5 1.868887-2 6.863380+5 6.270082-28325 684931579
 6.494200+5 2.600518-2 6.350200+5 4.448353-4 5.355280+5 7.551445-28325 684931580
 3.835880+5 4.803295-5 3.691880+5 2.852478-2 3.445240+5 8.478034-38325 684931581
 3.301240+5 5.327032-2 3.048960+5 2.083518-1 3.048800+5 1.577010-28325 684931582
 2.782400+5 6.935875-3 2.658320+5 4.898069-1 0.000000+0 0.000000+08325 684931583
 1.000000+0 0.000000+0                                        8325 684931584
 0.000000+0 2.000000+3         14          0        104         528325 684931585
 8.521680+5 5.085924-3 7.323380+5 1.732691-2 6.863380+5 5.766741-28325 684931586
 6.494200+5 2.409862-2 6.350200+5 4.126913-4 5.355280+5 6.982942-28325 684931587
 3.835880+5 4.451134-5 3.691880+5 2.646356-2 3.445240+5 7.856452-38325 684931588
 3.301240+5 4.942083-2 3.048960+5 1.931747-1 3.048800+5 1.460535-28325 684931589
 2.782400+5 6.453642-3 2.658320+5 4.528921-1 5.000000+2 1.271999-88325 684931590
 1.500000+3 1.296834-8 3.500000+3 1.371543-8 7.500000+3 1.496824-88325 684931591
 1.500000+4 1.750248-8 3.500000+4 2.682366-8 7.500000+4 3.947148-88325 684931592
 1.500000+5 1.562675-7 2.500000+5 8.169484-8 3.500000+5 9.229639-88325 684931593
 4.500000+5 6.190369-8 5.500000+5 4.169681-8 6.500000+5 2.742916-88325 684931594
 7.500000+5 2.159205-8 8.500000+5 7.887886-8 9.500000+5 4.612430-88325 684931595
 1.050000+6 3.173138-8 1.150000+6 2.692093-8 1.250000+6 1.302563-88325 684931596
 1.350000+6 7.538207-9 1.450000+6 5.288322-9 1.550000+6 3.411298-98325 684931597
 1.650000+6 2.071720-9 1.750000+6 1.180929-9 1.850000+6 6.42268-108325 684931598
 1.950000+6 4.12952-10 2.100000+6 1.61768-10 2.300000+6 5.01925-118325 684931599
 2.500000+6 1.78194-11 2.700000+6 5.05304-12 2.900000+6 1.50722-128325 684931600
 3.100000+6 4.18405-13 3.300000+6 7.77131-14 3.500000+6 2.43760-148325 684931601
 3.700000+6 3.48986-15 3.900000+6 3.67159-16 4.250000+6 1.00000-368325 684931602
 4.750000+6 1.00000-36                                        8325 684931603
```

The problem is caused by the continuum part of the energy spectrum: for the first few points (10^{-5}, 2.53 10^{-2} and 200 eV) this continuum is set to zero (there are only discrete photon lines). There are two solutions to the problem: either fix the evaluation (by replacing the zeros in the continuum by `1.00000-35`[1] [20]) or to propose a fix for NJOY to avoid this type of problem altogether (by replacing these zeros by `1.00000-35`).
This problem has been corrected for all library files of the Ti isotopes and ^{209}Bi included in this distribution.

[1]The problem remains when `1.00000-36` is used.

Chapter 5

Library QA - Validation

5.1 Introduction

Benchmarking the new libraries is a very important step in the development of a validated application library and must be as thorough and as complete as possible. The new libraries will be applied to a number of different fields: from thermal water moderated reactors, Accelerator Driven Systems (ADS) to shielding applications, ... Every application field has its specific demands on nuclear data. In thermal water moderated systems, the emphasis will lie on lower energy while ADS applications requires high energy data. Certain nuclides can be of significant importance in one application while they are not for another application. Accurate high energy data for Pb and Bi is for instance required for ADS applications, structural material data for shielding applications, ...
It is obvious that it is impossible to provide benchmarks for every possible material and application area so choices have to be made. We have therefore opted to perform a number of benchmark that were previously used to validate the standard MCNP libraries:

- criticality benchmarks which were already used for validating the MCNP ENDF60 and ENDF66 libraries
- the Lawrence Livermore pulsed sphere experiments

In order to be able to validate nuclear data, one must be sure that differences in benchmark results are really due to differences in data. Differences in library processing can introduce "noise" and is therefore not acceptable. Possible sources of such noise in a data library are different versions of NJOY (99.90, 99.90, 99.112, ...), different cross section reconstruction tolerances, ... This is why we decided to generate libraries for all major nuclear data evaluations available, all with the same basic set of NJOY input parameters.

5.2 Criticality Benchmarks

5.2.1 A Suite of Criticality Benchmarks for Validating Nuclear Data

In April 1999 Los ALamos National Laboratory released a suite of 86 criticality benchmarks [21] (along with the corresponding MCNP input files) for the specific purpose of validating nuclear data libraries for MCNP [22, 23]. We have decided to repeat these benchmarks for our newly generated MCNP(X) libraries.

The different benchmarks in the suite were specifically chosen to obtain a set of problems that would test different energy regions, such as the high-energy region of fast critical assemblies and the thermal region of the solution experiments, to test various reflector materials while maintaining an acceptable amount of benchmark problems.
This suite has been compiled using two compendiums of criticality experimental information: the Cross Section Evaluation Working Group (CSEWG) specifications and the International Criticality Safety Benchmark Evaluation Project (ICSBEP). The geometry and material specifications for the 86 benchmarks were taken primarily from the ICSBEP compendium.
In this suite, there are 5 different categories: critical assemblies with ^{233}U, intermediate enriched ^{235}U (IEU), highly enriched ^{235}U (HEU), ^{239}Pu and mixed metal assemblies (MM), see table 5.1. References to the CSEWG compendium in brackets indicate a corresponding set of CSEWG specifications that were not used in these benchmarks. Within every category there are bare, reflected and solution assemblies. The reflector materials themselves are Be, BeO, C, Al, Fe, Ni, W, Th, ^{233}U and natural uranium. For 5 assemblies there are two sets of specifications given so that we have to perform a total of 91 criticality calculations.

5.2.2 Benchmark Results

The numerical benchmark results for the criticality benchmarks can be found in table 5.2. This table includes the results for the ENDF60 and ENDF66 standard MCNP(X) libraries along with the results for the JEF 2.2, JEFF 3.0, JEFF 3.1, JENDL 3.3 and ENDF/B-VI.8 libraries included in ALEPH-LIB. Figure 5.1 plots these results with C/E (calculated over experimental) to visualise the tendencies in the results.

5.3 Lawrence Livermore Pulsed Sphere Benchmark

5.3.1 Experimental Setup

In the late 60's, Lawrence Livermore National Laboratory (LLNL) has performed a series of pulsed sphere experiments [24] to study neutron cross sections (both at low and high neutron energy) and for the purpose of validating neutron transport codes that were being used at LLNL (such as SORS and TART) [25, 26, 27, 28, 29, 30]. Los Alamos National Laboratory has also used these experiments to benchmark MCNP [31] and to benchmark ENDF/B-VI data [32, 33].
In these pulsed sphere experiments, an almost isotropic 14 MeV neutron source was placed at the center of a spherical target assembly. The resulting neutron emission spectra was then measured using time of flight techniques. For the high energy spectra, a total of 51 experiments on 38 different target configurations using 16 different materials have been performed (see table 5.3).
The nearly isotropic 14 MeV neutron source placed at the center of the spheres was produced by a T(d,n)^{4}He reaction. A deuteron beam was accelerated by the Livermore Insulated Core Transformer (ICT) accelerator to an energy of 400 keV and directed toward a tritiated titanium disk of 1.2 cm in diameter at the center of a cubical 40 ft. target pit. The target disk was held in place by a low mass structure made primarily of aluminum and stainless steel.
The neutron detectors (either the Pilot B or NE213 detector) that were used to measure the time-of-flight spectra were placed inside the target pit walls, behind collimators to protect them from the target pit background. Both the Pilot B and NE213 detector were operated at a 1.6 MeV neutron bias (neutrons below this energy were not detected). The neutrons detected have ener-

Table 5.1: Criticality benchmark descriptions.

Name	Type	Description	CSEWG	ICSBEP
23umt1	^{233}U	Jezebel-23, Bare Sphere of U233	(F-19)	233U-MET-FAST-001
23umt2a	^{233}U	0.481" HEU-Reflected Sphere of U233; Planet Assembly		233U-MET-FAST-002 Case 1
23umt2b	^{233}U	0.783" HEU-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-002 Case 2
23umt3a	^{233}U	0.906" Normal Uranium-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-003 Case 1
23umt3b	^{233}U	2.09" Normal Uranium-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-003 Case 2
23umt4a	^{233}U	0.96" Tungsten-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-004 Case 1
23umt4b	^{233}U	2.28" Tungsten-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-004 Case 2
23umt5a	^{233}U	0.805" Be-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-005 Case 1
23umt5b	^{233}U	1.652" Be-Reflected Sphere of U233, Planet Assembly		233U-MET-FAST-005 Case 2
23umt6	^{233}U	Flattop-23, 7.84" Normal-Uranium Reflected Sphere of U233		233U-MET-FAST-006
flat23	^{233}U	Flattop-23, CSEWG, U(N)-reflected U233 sphere + gap	F-24	
23usl1a	^{233}U	ORNL-5, 1.0226 g/l Unreflected 27.24" Sphere of U233 nitrate solution		233U-SOL-THERM-001 Case 1
23usl1b	^{233}U	ORNL-6, 1.0253 g/l Unreflected 27.24" Sphere of U233 nitrate solution with Boron		233U-SOL-THERM-001 Case 2
23usl1c	^{233}U	ORNL-7, 1.0274 g/l Unreflected 27.24" Sphere of U233 nitrate solution with Boron		233U-SOL-THERM-001 Case 3
23usl1d	^{233}U	ORNL-8, 1.0275 g/l Unreflected 27.24" Sphere of U233 nitrate solution with Boron		233U-SOL-THERM-001 Case 4
23usl1e	^{233}U	ORNL-9, 1.0286 g/l Unreflected 27.24" Sphere of U233 nitrate solution with Boron		233U-SOL-THERM-001 Case 5
23usl8	^{233}U	ORNL-11, 1.0153 g/l Unreflected 48.04" Sphere of U233 nitrate solution with Boron		233U-SOL-THERM-008
ieumt1a	IEU	Jemima 1, Cylindrical Disks of HEU and Natural Uranium		IEU-MET-FAST-001 Case 1
ieumt1b	IEU	Jemima 2, Cylindrical Disks of HEU and Natural Uranium		IEU-MET-FAST-001 Case 2
ieumt1c	IEU	Jemima 3, Cylindrical Disks of HEU and Natural Uranium		IEU-MET-FAST-001 Case 3

Continued on next page

Name	Type	Description	CSEWG	ICSBEP
ieumt1d	IEU	Jemima 4, Cylindrical Disks of HEU and Natural Uranium		IEU-MET-FAST-001 Case 4
ieumt2	IEU	Reflected Jemima, U(N)-Reflected Cylindrical Disks of HEU and Natural Uranium		IEU-MET-FAST-002
ieumt3	IEU	Bare IEU Sphere (36 wt.%), VNIIEF		IEU-MET-FAST-003
ieumt4	IEU	Graphite-Reflected IEU Sphere (36 wt.%), VNIIEF		IEU-MET-FAST-004
ieumt5	IEU	Steel-Reflected IEU Sphere (36 wt.%), VNIIEF		IEU-MET-FAST-005
ieumt6	IEU	Duralumin-Reflected IEU Sphere (36 wt.%), VNIIEF		IEU-MET-FAST-006
umet1ss	HEU	Godiva, Unreflected sphere of HEU, Simple Sphere representation	(F-5)	HEU-MET-FAST-001 Case a
umet1ns	HEU	Godiva, Unreflected sphere of HEU, Nested Spherical shell representation		HEU-MET-FAST-001 Case b
bigten1	HEU	BIGTEN, 1d model: U(N) reflected uranium sphere	F-10	
bigten2	HEU	BIGTEN, 2d model: U(N) reflected uranium cylinder		
umet3a	HEU	2" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 1
umet3b	HEU	3" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 2
umet3c	HEU	4" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 3
umet3d	HEU	5" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 4
umet3e	HEU	7" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 5
umet3f	HEU	8" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 6
umet3g	HEU	11" Tuballoy-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 7
umet3h	HEU	1.9" Tungsten Carbide-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 8
umet3i	HEU	2.9" Tungsten Carbide-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 9
umet3j	HEU	4.5" Tungsten Carbide-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 10
umet3k	HEU	6.5" Tungsten Carbide-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 11
umet3l	HEU	8.0" Nickel-Reflected HEU(93.5) Sphere, Topsy Assembly		HEU-MET-FAST-003 Case 12
umet4a	HEU	Water-Reflected HEU(97.675) Sphere, with plexiglass ring		HEU-MET-FAST-004 Case 2
umet4b	HEU	Water-Reflected HEU(97.675) Sphere, Trans. Am. Nuc. Soc. 27, pg. 412 (1977)		HEU-MET-FAST-004 (Case 1)
umet8	HEU	Bare HEU Sphere, VNIITF, 3D model		HEU-MET-FAST-008
umet9a	HEU	Be-Reflected HEU(89.6) Sphere, VNIITF		HEU-MET-FAST-009 Case 1

Continued on next page

Name	Type	Description	CSEWG	ICSBEP
umet9b	HEU	BeO-Reflected HEU(89.6) Sphere, VNIITF		HEU-MET-FAST-009 Case 2
umet11	HEU	Polyethylene (CH2)-Reflected HEU(89.6) Sphere, VNIITF		HEU-MET-FAST-011
umet12	HEU	Aluminium-Reflected HEU(89.6) Sphere, VNIITF		HEU-MET-FAST-012
umet13	HEU	St.20 Steel-Reflected HEU(89.6) Sphere, VNIITF		HEU-MET-FAST-013
umet14	HEU	Depleted Uranium-Reflected HEU(89.6) Sphere, VNIITF		HEU-MET-FAST-014
umet15	HEU	Bare HEU Cylinder, VNIITF		HEU-MET-FAST-015
umet18	HEU	Simplified Bare HEU Sphere, VNIIEF		HEU-MET-FAST-018
umet19	HEU	Graphite-Reflected HEU Sphere, VNIIEF		HEU-MET-FAST-019
umet20	HEU	Polyethylene-Reflected HEU Sphere, VNIIEF		HEU-MET-FAST-020
umet21	HEU	Steel-Reflected HEU Sphere, VNIIEF		HEU-MET-FAST-021
umet22	HEU	Duralumin-Reflected HEU Sphere, VNIIEF		HEU-MET-FAST-022
umet28	HEU	Flattop-25, U(nat)-Reflected HEU SPHERE	(F-22)	HEU-MET-FAST-028
usol13a	HEU	ORNL-1, Unreflected Sphere of Uranyl(20.12 g/l) Nitrate	(T-1)	HEU-SOL-THERM-003 Case 1
usol13b	HEU	ORNL-2, Unreflected Sphere of Uranyl(23.53 g/l) Nitrate with Boron	(T-2)	HEU-SOL-THERM-003 Case 2
usol13c	HEU	ORNL-3, Unreflected Sphere of Uranyl(26.77 g/l) Nitrate with Boron	(T-3)	HEU-SOL-THERM-003 Case 3
usol13d	HEU	ORNL-4, Unreflected Sphere of Uranyl(28.45 g/l) Nitrate with Boron	(T-4)	HEU-SOL-THERM-003 Case 4
usol32	HEU	ORNL-10, Unreflected Sphere of Uranyl(28.45 g/l) Nitrate with Boron	(T-5)	HEU-SOL-THERM-032
pumet1	^{239}Pu	Jezebel-Pu (4.5 %), Bare sphere of Pu-239 with 4.5 % Pu-240	(F-1)	PU-MET-FAST-001
pumet2	^{239}Pu	Jezebel-Pu (20 %), Bare sphere of Pu-239 with 20 % Pu-240	(F-21)	PU-MET-FAST-002
pumet5	^{239}Pu	Tungsten-Reflected Pu(94.79) Sphere, Planet assembly		PU-MET-FAST-005
pumet6	^{239}Pu	Normal Uranium-Reflected Pu(93.80) Sphere, Flattop assembly	(F-23)	PU-MET-FAST-006
pumet8a	^{239}Pu	Thorium-Reflected Pu(93.59) Sphere, Thor Assembly, 1D Model	(F-25)	PU-MET-FAST-008 Case 1
pumet8b	^{239}Pu	Thorium-Reflected Pu(93.59) Sphere, Thor Assembly, 2D Model		PU-MET-FAST-008 Case 2
pumet9	^{239}Pu	Aluminum-Reflected Pu(94.8) Sphere, Comet Assembly		PU-MET-FAST-009
pumet10	^{239}Pu	U(N)-Reflected Pu sphere		PU-MET-FAST-010
pumet11	^{239}Pu	Water-Reflected alpha-phase Pu sphere		PU-MET-FAST-011
pumet18	^{239}Pu	Be-Reflected Pu(94.79) Sphere, Planet Assembly		PU-MET-FAST-018
pumet19	^{239}Pu	Be-Reflected Pu(90) Sphere, VNIITF		PU-MET-FAST-019
pumet20	^{239}Pu	Depleted Uranium-Reflected Pu(90) Sphere, VNIITF		PU-MET-FAST-020

Continued on next page

Name	Type	Description	CSEWG	ICSBEP
pumt21a	^{239}Pu	Be-Reflected Pu Cylinder		PU-MET-FAST-021 Case 1
pumt21b	^{239}Pu	BeO-Reflected Pu Cylinder		PU-MET-FAST-021 Case 2
pumet22	^{239}Pu	Simplified Plutonium (98 %)Bare Sphere, VNIIEF		PU-MET-FAST-022
pumet23	^{239}Pu	Simplified Plutonium Sphere, Graphite reflector, VNIIEF		PU-MET-FAST-023
pumet24	^{239}Pu	Simplified Plutonium Sphere, Polyethylene Reflector, VNIIEF		PU-MET-FAST-024
pumet25	^{239}Pu	Simplified Plutonium Sphere, 1.55 cm Steel Reflector, VNIIEF		PU-MET-FAST-025
pumet26	^{239}Pu	Simplified Plutonium Sphere, 11.9 cm Steel Reflector, VNIIEF		PU-MET-FAST-026
pnl1	^{239}Pu	PNL-1, Idealized (No Container) Unreflected Sphere of Pu Nitrate Solution	T-13	
pnl6	^{239}Pu	PNL-6, Idealized (No Container) Unreflected Sphere of Pu Nitrate Solution; Revised PNL2	T-14,T-24	
pusl11a	^{239}Pu	PNL-3, Unreflected 18" Sphere of Pu(22.35 g/l) Nitrate Solution	(T-15)	PU-SOL-THERM-011 Case 18-1
pusl11b	^{239}Pu	PNL-4, Unreflected 18" Sphere of Pu(27.49 g/l) Nitrate Solution	(T-16)	PU-SOL-THERM-011 Case 18-6
pusl11c	^{239}Pu	PNL-5, Unreflected 16" Sphere of Pu(43.43g/l) Nitrate Solution	(T-17)	PU-SOL-THERM-011 Case 16-5
pusl11d	^{239}Pu	Unreflected 16" Sphere of Pu(34.96g/l) Nitrate Solution		PU-SOL-THERM-011 Case 16-1
mixmet1	MM	HEU-Reflected Pu Sphere, Planet Assembly		MIX-MET-FAST-001
mixmet3	MM	HEU-Reflected Pu Sphere, VNIITF		MIX-MET-FAST-003
mixmet8	MM	ZEBRA 8A/2, Graphite and Natural Uranium reflected Pu		MIX-MET-FAST-008 Case 1

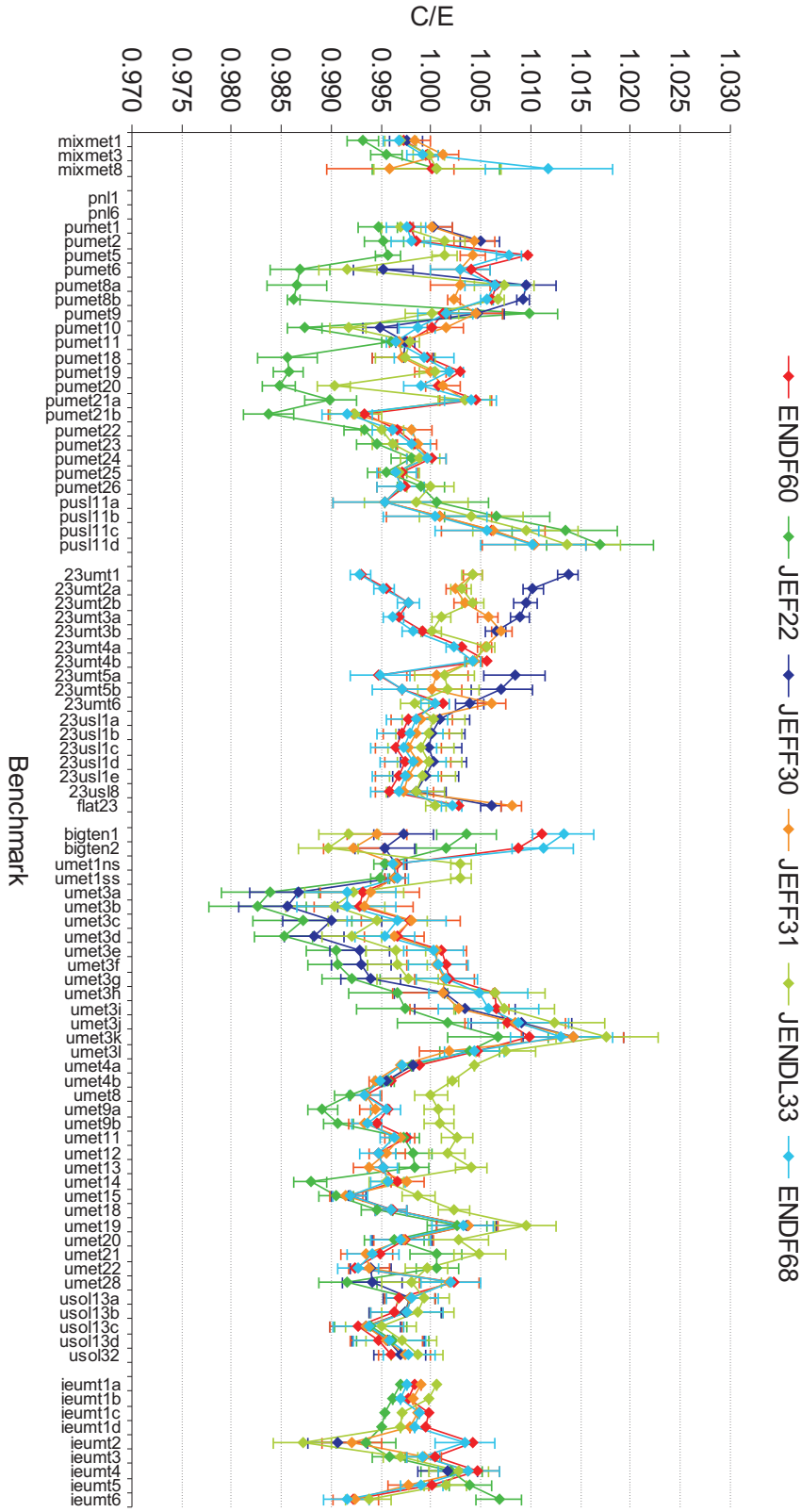

Figure 5.1: C/E results for the criticality benchmarks.

Table 5.2: Criticality benchmark results.

Name	Result	ENDF60	ENDF66	JEF 2.2	JEFF 3.0	JEFF 3.1	JENDL 3.3	ENDF/B-VI.8
mixmet1	1.00000 (160)	0.99722 (12)	0.99683 (12)	0.99320 (12)	0.99750 (12)	0.99833 (12)	0.99698 (11)	0.99675 (11)
mixmet3	0.99930 (160)	0.99883 (12)	0.99826 (11)	0.99479 (11)	-	1.00042 (12)	0.99906 (12)	0.99842 (11)
mixmet8	0.99200 (630)	0.99214 (10)	1.00433 (10)	0.99247 (9)	-	0.98792 (10)	0.99261 (9)	1.00367 (9)
pnl1	-	1.00818 (12)	1.00879 (12)	1.01499 (12)	1.00862 (12)	1.00821 (12)	1.01123 (12)	1.00767 (12)
pnl6	-	1.00327 (13)	1.00354 (14)	1.01074 (14)	1.00453 (13)	1.00352 (13)	1.00655 (13)	1.00243 (14)
pumet1	1.00000 (200)	0.99781 (11)	0.99750 (11)	0.99468 (11)	1.00019 (12)	1.00012 (11)	0.99698 (11)	0.99751 (11)
pumet2	1.00000 (200)	0.99853 (11)	0.99805 (11)	0.99523 (11)	1.00490 (12)	1.00435 (11)	1.00131 (11)	0.99798 (11)
pumet5	1.00000 (130)	1.00964 (12)	1.00770 (12)	0.99564 (12)	-	1.00416 (12)	1.00131 (12)	1.00780 (12)
pumet6	1.00000 (300)	1.00396 (14)	1.00253 (14)	0.98688 (14)	0.99526 (13)	1.00297 (13)	0.99165 (14)	1.00289 (14)
pumet8a	1.00000 (300)	1.00658 (13)	1.00666 (12)	0.98654 (12)	1.00945 (12)	1.00294 (12)	1.00734 (13)	1.00635 (12)
pumet8b	1.00000 (60)	1.00603 (12)	1.00574 (12)	0.98623 (11)	1.00915 (12)	1.00234 (12)	1.00672 (12)	1.00555 (12)
pumet9	1.00000 (270)	1.00111 (12)	1.00114 (12)	1.00987 (12)	1.00463 (12)	1.00448 (12)	1.00005 (12)	1.00142 (12)
pumet10	1.00000 (180)	1.00014 (12)	0.99866 (12)	0.98734 (12)	0.99487 (11)	1.00147 (12)	0.99168 (11)	0.99859 (12)
pumet11	1.00000 (100)	0.99753 (14)	0.99695 (14)	0.99603 (14)	0.99741 (14)	0.99681 (15)	0.99788 (15)	0.99648 (13)
pumet18	1.00000 (300)	0.99968 (12)	0.99917 (12)	0.98555 (12)	0.99717 (13)	0.99705 (12)	0.99746 (13)	0.99929 (12)
pumet19	0.99920 (150)	1.00208 (12)	1.00126 (13)	0.98491 (12)	-	0.99913 (13)	0.99959 (13)	1.00095 (12)
pumet20	0.99930 (170)	1.00002 (12)	0.99848 (13)	0.98406 (13)	-	1.00050 (12)	0.98956 (13)	0.99830 (12)
pumet21a	1.00000 (260)	1.00452 (13)	1.00407 (12)	0.98989 (12)	-	1.00346 (13)	1.00332 (13)	1.00397 (13)
pumet21b	1.00000 (260)	0.99324 (12)	0.99252 (13)	0.98370 (12)	-	0.99220 (13)	0.99242 (12)	0.99157 (13)
pumet22	1.00000 (210)	0.99658 (11)	0.99614 (12)	0.99333 (11)	-	0.99804 (11)	0.99510 (11)	0.99615 (11)
pumet23	1.00000 (200)	0.99829 (11)	0.99786 (12)	0.99449 (12)	-	0.99862 (12)	0.99616 (12)	0.99796 (12)
pumet24	1.00000 (200)	1.00002 (12)	0.99986 (13)	0.99804 (12)	-	0.99954 (13)	0.99887 (13)	0.99954 (13)
pumet25	1.00000 (200)	0.99709 (11)	0.99659 (12)	0.99556 (12)	-	0.99665 (11)	0.99682 (12)	0.99653 (12)
pumet26	1.00000 (240)	0.99742 (12)	0.99663 (12)	0.99901 (12)	-	0.99697 (12)	0.99993 (12)	0.99694 (12)
pusl11a	1.00000 (520)	0.99543 (10)	0.99617 (10)	1.00061 (10)	-	0.99541 (10)	0.99851 (11)	0.99536 (11)
pusl11b	1.00000 (520)	1.00080 (11)	1.00132 (11)	1.00658 (11)	-	1.00079 (11)	1.00406 (11)	1.00046 (11)
pusl11c	1.00000 (520)	1.00612 (12)	1.00648 (12)	1.01339 (12)	-	1.00618 (12)	1.00948 (12)	1.00561 (12)

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Name	Result	ENDF60	ENDF66	JEF 2.2	JEFF 3.0	JEFF 3.1	JENDL 3.3	ENDF/B-VI.8
pusl11d	1.00000 (520)	1.01031 (12)	1.01107 (12)	1.01692 (12)	-	1.01032 (12)	1.01364 (12)	1.01018 (12)
23umt1	1.00000 (100)	0.99307 (11)	0.99287 (11)	-	1.01371 (11)	1.00416 (11)	1.00412 (11)	0.99288 (10)
23umt2a	1.00000 (100)	0.99559 (11)	0.99521 (11)	-	1.01023 (12)	1.00251 (12)	1.00302 (12)	0.99527 (12)
23umt2b	1.00000 (110)	0.99766 (11)	0.99742 (11)	-	1.00945 (12)	1.00343 (12)	1.00422 (11)	0.99770 (11)
23umt3a	1.00000 (100)	0.99681 (11)	0.99618 (11)	-	1.00890 (12)	1.00567 (12)	1.00102 (12)	0.99622 (11)
23umt3b	1.00000 (100)	0.99916 (11)	0.99823 (12)	-	1.00646 (12)	1.00707 (13)	1.00005 (12)	0.99813 (12)
23umt4a	1.00000 (70)	1.00303 (12)	1.00207 (12)	-	-	1.00542 (11)	1.00561 (12)	1.00222 (12)
23umt4b	1.00000 (80)	1.00561 (13)	1.00418 (12)	-	-	1.00429 (12)	1.00421 (12)	1.00414 (12)
23umt5a	1.00000 (300)	0.99468 (12)	0.99483 (11)	-	1.00835 (12)	1.00062 (12)	1.00137 (12)	0.99494 (13)
23umt5b	1.00000 (300)	0.99708 (12)	0.99721 (13)	-	1.00704 (13)	1.00010 (13)	1.00172 (13)	0.99713 (12)
23umt6	1.00000 (140)	1.00124 (13)	1.00036 (13)	-	1.00389 (13)	1.00610 (13)	0.99834 (13)	1.00033 (13)
23usl1a	1.00000 (310)	0.99777 (8)	0.99876 (7)	-	1.00081 (8)	0.99903 (7)	1.00024 (8)	0.99853 (7)
23usl1b	1.00050 (330)	0.99755 (8)	0.99776 (7)	-	1.00054 (8)	0.99902 (7)	1.00021 (7)	0.99839 (7)
23usl1c	1.00060 (330)	0.99705 (8)	0.99819 (8)	-	1.00031 (8)	0.99834 (8)	0.99955 (8)	0.99783 (8)
23usl1d	0.99980 (330)	0.99722 (8)	0.99817 (8)	-	1.00010 (8)	0.99848 (8)	0.99964 (8)	0.99800 (8)
23usl1e	0.99990 (330)	0.99673 (8)	0.99758 (8)	-	0.99934 (8)	0.99761 (8)	0.99899 (8)	0.99727 (8)
23usl8	1.00060 (290)	0.99640 (5)	0.99749 (5)	-	0.99913 (5)	0.99788 (5)	0.99903 (5)	0.99739 (5)
flat23	1.00000 (100)	1.00281 (13)	1.00216 (13)	-	1.00601 (13)	1.00808 (13)	1.00042 (13)	1.00209 (13)
bigten1	0.99600 (300)	1.00706 (10)	1.00941 (9)	0.99956 (10)	0.99329 (9)	0.99052 (10)	0.98784 (10)	1.00918 (10)
bigten2	0.99600 (300)	1.00465 (10)	1.00736 (10)	0.99754 (9)	0.99136 (9)	0.98819 (9)	0.98569 (10)	1.00718 (10)
umet1ns	1.00000 (100)	0.99656 (12)	0.99645 (11)	0.99529 (11)	0.99653 (11)	0.99639 (12)	1.00296 (11)	0.99619 (12)
umet1ss	1.00000 (100)	0.99655 (11)	0.99647 (11)	0.99490 (11)	0.99633 (11)	0.99637 (12)	1.00294 (11)	0.99668 (11)
umet3a	1.00000 (500)	0.99308 (12)	0.99170 (11)	0.98383 (12)	0.98667 (12)	0.99387 (12)	0.99225 (11)	0.99154 (12)
umet3b	1.00000 (500)	0.99276 (11)	0.99180 (12)	0.98259 (12)	0.98566 (12)	0.99328 (12)	0.99036 (12)	0.99156 (11)
umet3c	1.00000 (500)	0.99792 (12)	0.99686 (12)	0.98710 (11)	0.99005 (12)	0.99796 (12)	0.99464 (12)	0.99654 (12)
umet3d	1.00000 (300)	0.99664 (12)	0.99523 (12)	0.98522 (12)	0.98823 (11)	0.99625 (12)	0.99210 (12)	0.99531 (12)
umet3e	1.00000 (300)	1.00106 (13)	1.00028 (12)	0.99048 (13)	0.99283 (12)	1.00051 (12)	0.99642 (12)	1.00020 (13)
umet3f	1.00000 (300)	1.00156 (12)	1.00066 (13)	0.99067 (13)	0.99306 (12)	1.00055 (13)	0.99665 (12)	1.00073 (12)
umet3g	1.00000 (300)	1.00183 (13)	1.00142 (13)	0.99198 (12)	0.99387 (13)	1.00137 (13)	0.99764 (12)	1.00156 (13)

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Name	Result	ENDF60	ENDF66	JEF 2.2	JEFF 3.0	JEFF 3.1	JENDL 3.3	ENDF/B-VI.8
umet3h	1.00000 (500)	1.00635 (12)	1.00464 (12)	0.99665 (12)	1.00133 (12)	1.00115 (13)	1.00645 (12)	1.00473 (12)
umet3i	1.00000 (500)	1.00656 (13)	1.00582 (12)	0.99748 (12)	1.00341 (12)	1.00283 (12)	1.00738 (12)	1.00581 (13)
umet3j	1.00000 (500)	1.00768 (12)	1.00917 (12)	1.00165 (12)	1.00902 (12)	1.00843 (12)	1.01233 (12)	1.00870 (12)
umet3k	1.00000 (500)	1.00985 (12)	1.01351 (12)	1.00668 (12)	1.01421 (13)	1.01418 (13)	1.01763 (13)	1.01306 (12)
umet3l	1.00000 (300)	1.00468 (12)	1.00433 (12)	1.00385 (12)	-	1.00175 (12)	1.00746 (12)	1.00431 (12)
umet4a	1.00200	1.00082 (14)	0.99961 (15)	1.00008 (14)	1.00012 (14)	0.99893 (14)	1.00637 (15)	0.99906 (14)
umet4b	1.00030 (50)	0.99634 (15)	0.99578 (15)	0.99601 (15)	0.99584 (14)	0.99466 (14)	1.00249 (14)	0.99511 (14)
umet8	0.99890 (160)	0.99243 (11)	0.99221 (12)	0.99077 (12)	-	0.99242 (11)	0.99887 (11)	0.99223 (11)
umet9a	0.99920 (150)	0.99482 (13)	0.99505 (13)	0.98833 (12)	-	0.99354 (12)	0.99995 (12)	0.99465 (12)
umet9b	0.99920 (150)	0.99381 (12)	0.99363 (12)	0.98985 (12)	-	0.99244 (12)	0.99999 (11)	0.99282 (12)
umet11	0.99890 (150)	0.99645 (15)	0.99513 (14)	0.99619 (15)	-	0.99581 (15)	1.00149 (14)	0.99525 (14)
umet12	0.99920 (180)	0.99391 (12)	0.99380 (12)	0.99742 (12)	-	0.99476 (11)	1.00082 (12)	0.99387 (12)
umet13	0.99900 (150)	0.99418 (11)	0.99405 (12)	0.99731 (12)	-	0.99271 (11)	1.00302 (11)	0.99418 (12)
umet14	0.99890 (170)	0.99553 (12)	0.99433 (12)	0.98682 (11)	-	0.99653 (12)	0.99443 (12)	0.99457 (12)
umet15	0.99960 (170)	0.99150 (12)	0.99109 (11)	0.99007 (12)	0.99133 (11)	0.99106 (12)	0.99832 (12)	0.99149 (12)
umet18	1.00000 (160)	0.99616 (11)	0.99605 (12)	0.99454 (11)	0.99602 (11)	0.99601 (12)	1.00224 (11)	0.99600 (12)
umet19	1.00000 (300)	1.00364 (12)	1.00344 (12)	1.00254 (12)	1.00353 (12)	1.00363 (12)	1.00948 (12)	1.00317 (12)
umet20	1.00000 (300)	0.99741 (13)	0.99658 (13)	0.99628 (13)	0.99708 (13)	0.99724 (13)	1.00278 (12)	0.99687 (13)
umet21	1.00000 (260)	0.99488 (12)	0.99401 (12)	1.00054 (11)	-	0.99351 (12)	1.00485 (11)	0.99415 (11)
umet22	1.00000 (210)	0.99230 (12)	0.99238 (11)	1.00060 (12)	0.99397 (12)	0.99380 (12)	0.99955 (11)	0.99264 (12)
umet28	1.00000 (300)	1.00235 (13)	1.00183 (13)	0.99164 (12)	0.99416 (13)	1.00181 (12)	0.99800 (12)	1.00195 (12)
usol13a	1.00120 (260)	0.99789 (8)	0.99953 (7)	0.99904 (7)	0.99906 (7)	0.99907 (7)	1.00043 (7)	0.99930 (7)
usol13b	1.00070 (360)	0.99700 (8)	0.99850 (8)	0.99814 (8)	0.99813 (8)	0.99826 (8)	0.99941 (8)	0.99829 (8)
usol13c	1.00090 (360)	0.99357 (8)	0.99487 (9)	0.99482 (9)	0.99428 (8)	0.99439 (8)	0.99587 (8)	0.99464 (8)
usol13d	1.00030 (360)	0.99506 (9)	0.99648 (8)	0.99643 (8)	0.99598 (8)	0.99580 (9)	0.99732 (9)	0.99610 (8)
usol32	1.00150 (260)	0.99749 (6)	0.99915 (6)	-	0.99840 (5)	0.99886 (5)	1.00015 (5)	0.99923 (6)
ieumt1a	0.99890	0.99723 (12)	0.99677 (11)	0.99577 (12)	-	0.99786 (12)	0.99944 (11)	0.99652 (12)
ieumt1b	0.99970	0.99743 (12)	0.99673 (12)	0.99579 (12)	-	0.99796 (11)	0.99947 (12)	0.99666 (12)
ieumt1c	0.99930	0.99908 (12)	0.99785 (12)	0.99472 (12)	-	0.99794 (12)	0.99643 (11)	0.99812 (11)

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Name	Result	ENDF60	ENDF66	JEF 2.2	JEFF 3.0	JEFF 3.1	JENDL 3.3	ENDF/B-VI.8
ieumt1d	1.00020	0.99964 (12)	0.99824 (12)	0.99516 (13)	-	0.99810 (11)	0.99711 (11)	0.99855 (13)
ieumt2	1.00000 (300)	1.00419 (11)	1.00347 (10)	0.99353 (11)	0.99066 (10)	0.99209 (11)	0.98710 (11)	1.00335 (11)
ieumt3	1.00000 (170)	1.00046 (12)	0.99893 (12)	0.99577 (11)	-	0.99926 (12)	0.99692 (12)	0.99920 (11)
ieumt4	1.00000 (300)	1.00465 (11)	1.00381 (12)	1.00204 (12)	1.00169 (12)	1.00376 (12)	1.00279 (12)	1.00376 (12)
ieumt5	1.00000 (210)	1.00010 (12)	0.99883 (11)	1.00388 (12)	-	0.99771 (12)	1.00146 (11)	0.99901 (12)
ieumt6	1.00000 (230)	0.99217 (11)	0.99117 (12)	1.00678 (11)	-	0.99241 (12)	0.99374 (11)	0.99154 (12)

Table 5.3: Target material overview for the Lawrence Livermore pulsed sphere experiments.

Material	Size	Experiment	Material	Size	Experiment
^{6}Li	0.5	01, 02	Ti	1.2	28
	1.1	03		2.2	29
	1.6	04		3.5	30
^{7}Li	0.5	05, 06	Fe	0.9	31, 32
	1.1	07		2.9	33, 34
	1.6	08		4.8	35, 36
Be	0.8	09	Pb	1.4	37, 38
C	0.5	10, 11	H_2O	1.1	39
	1.3	12, 13		1.9	40, 41
	2.9	14, 15	D_2O	1.2	42
N	1.1	17		2.1	43
	3.1	18	Polyethylene	0.7	44
O	1.1	19		1.6	45
Mg	0.7	20, 21		3.0	46
	1.2	22	Teflon	0.9	47
	1.9	23		1.8	48
Al	0.9	24, 25		2.9	49, 50
	1.6	26	Concrete	2.0	52
	2.6	27		3.8	54

gies ranging from about 16 MeV to 2 MeV. As such, the pulsed sphere experiments described here are excellent benchmarks for the higher energy cross sections (above 2 MeV).
The detectors were placed at 30 degrees and 120 degrees with respect to the beam line at distance between 750 and 925 cm (depending on the angle used and the experiment). A measurement at 30 degrees was made for every type of sphere and material. Only those spheres and materials that have two experiment numbers in table 5.3 have measurements at 120 degrees.
The pulsed sphere experiments are a lot more sensitive to cross section data and even angular distributions when compared to integral benchmarks (a very good example are the magnesium spheres, see section 5.3.3 and figures 5.22 to 5.25). This aspect alone makes them prime candidates for validating nuclear data because even the smallest differences will be very clear.
In general, the following requirements must be met to obtain agreement between the experimental time of flight spectrum and those obtained through calculations:

- the correct total and total elastic cross section at around 15 MeV (the transmitted peak and the elastic region is sensitive to cross sections at that energy)
- the correct total cross section over the entire energy range
- the correct total and level inelastic scattering cross sections
- the correct angular distribution for elastic scattering and the levels of inelastic scattering

The neutron source itself (in particular the energy and angle distribution) must be well known because the position of the transmitted peak is determined by the neutron energy of the source under the measured angle. This has however nothing to do with the nuclear data itself. This

neutron source must be modeled correctly in the transport code that is used (something which has already been done by LANL [32, 33]).

5.3.2 MCNPX Calculations

As mentioned before, the pulsed sphere experiments can be used to benchmark both neutron cross section data and neutron transport codes. In general these two aspects cannot be separated, but they are separable when the relevant neutron cross sections are accurately known or when we are satisfied from other considerations that the neutron transport code being used is correct. In our case, we want to benchmark different nuclear data evaluations using MCNPX 2.5.e, a code of which the validity has been proven on numerous occasions.
Some of these pulsed sphere experiments have already been used for benchmarks with MCNP [31, 33]. These reports also included the MCNP input files that were used for those benchmarks. Because not every pulsed sphere experiment from the original LLNL report [24] is given in the previously mentioned LANL reports, we have decided to remodel the geometry of every pulsed sphere experiment as it was given in the original LLNL report. The MCNP(X) input files for these revised geometries are detailed in [34].
The experimental data from the LLNL report [24] is expressed as counts per ns per source particle (detected neutrons at the detector when the target sphere is not present). As such, the calculated time of flight spectrum must be divided by 2 (because we use 2 ns time bins) and by the total number of neutrons that reach the detector when the target sphere is not present (this requires a seperate calculation).
Using this normalised time of flight spectrum we have also integrated the number of counts in time bins corresponding with neutron energies of 12-16 MeV and 2-16 MeV. Determination of the time bins was based on the time a particle of a given energy would take to travel from the center of the sphere to the detector without collision (the LLNL report contains this information for every target sphere).
The calculations were all run to obtain an accuracy of 0.1 % on the total value. This way, the error in every 2 ns time bin (except for the first few time bins) is equal to or below 1 %. In most cases, this could be achieved with 20 million neutron particles when no variance reduction techniques were used. The calculation time itself varied from 20 min per sphere (e.g. the ^{9}Be calculations) to 2 hours (e.g. the Pb calculations) on a 3 GHz CPU. An exception to this are the Fe calculations which used 8 times more particles to obtain the proper accuracy and about 10 hours to complete.

5.3.3 Benchmark Results and Discussion

Figures 5.4 to 5.54 (at the end of this chapter) give the results for the 51 pulsed sphere experiments that can be found in the original LLNL report [24]. For every sphere, we have calculated the time of flight spectrum using the standard MCNP(X) libraries ENDF60 and ENDF66 and all the libraries contained in ALEPH-LIB (JEF 2.2, JEFF 3.0, JEFF 3.1, JENDL 3.3 and ENDF/B-VI.8). For each experiment, there is an overview graph of all results along with 7 other graphs for each individual result (making it a lot easier to compare with the experiment itself). Whenever an evaluation required for the calculation was missing from the ace libraries, the figure will contain the text “No result due to missing evaluation.”.

Lithium spheres

We start with 8 experiments on lithium spheres (four with ^{6}Li and another four with ^{6}Li) in figures 5.4 to 5.11. There are three configurations for these lithium spheres (with radii of 8.97, 16.52 and 25.52 cm) where the different parts are encased in a metal cladding (68.6% Fe, 20.0% Cr, 8.4% Ni, 2.0% Si and 1.0% Mn). It should be noted that the density of the casing was rather high when compared to other spheres that use the same casing material (> 9.0 g cm^{-3} compared to the usual 7.9 g cm^{-3}). In our calculations, we have used those high values in order to conserve the mass of the material.
The JEFF 3.0 library is missing one of the isotopes (^{60}Ni) in the cladding so no results are presented for this library (the cladding can have significant impact on the results, we refer to the case of liquid oxygen for an obvious example). Fortunately, the lithium data in JEFF 3.0 is taken over in JEFF 3.1 so that differences between both libraries would only be due to different data for the casing materials. In the ^{6}Li) graphs, we can also see that the JEFF 3.1 and ENDF/B-VI.8 curves are (practically) the same. In this case, the time of flight spectrum is dominated by the lithium (contrary to the liquid oxygen sphere where the casing has a larger influence).
For the ^{6}Li spheres it is rather difficult to draw a conclusion. There are three families of curves: ENDF (ENDF/B-VI.8 and JEFF 3.1 have the same lithium data), JENDL 3.3 and JEF 2.2. All families seem to be good in the transmitted peak. But beyond the transmitted peak, they tend to separate (first JEF 2.2 and later on JENDL 3.3). In that region, JENDL 3.3 followed by JEF 2.2 appear to be the best. At the end of the time of flight spectrum, the JEF 2.2 curve joins the ENDF curves. And in that region, the JEF 2.2 and ENDF curves appear to be the best.
The situation is however very different for the ^{7}Li spheres. The curves for the different libraries are already a lot closer to each other. The JEFF 3.1 evaluation (taken from JEFF 3.0 which in turn took the data from an EFF 2.4 evaluation) and JENDL 3.3 appear to be the best, closely followed by ENDF/B-VI.8 and JEF 2.2 (based on an older EFF evaluation).

The beryllium sphere

The results for a beryllium sphere can be found in figure 5.12. In this case, it is a hollow sphere with an outer diameter of 12.58 cm and inner diameter of 8 cm.
There are again three different tendencies in the results: ENDF (JENDL 3.3 is very close to the ENDF curves although there is no relation between the two), JEFF and JEF 2.2. From the graphs, it is obvious that the JEF 2.2 curve is completely off (by at least a factor 2). Just as with the lithium spheres, it is not so simply to draw a definite conclusion here. Just beyond the transmitted peak, JEFF 3.1 appears to be the best. In the middle of the time of flight spectrum it appears to be ENDF while at the end JENDL 3.3 is the closest.
As noted in chapter 4, the JEFF 3.0 data (based on EFF 3.0 mod 2) had to be corrected because NJOY added the (n,2n) reaction twice. It appears that NJOY does not distinguish between mt16 (total (n,2n)) and mt875 to 890 (the different levels of the (n,2n) reaction). The JEFF 3.1 file was also based on EFF 3.0 evaluation (mod 6), but this file already had this correction. This (n,2n) problem is also clearly visible in the beryllium pulsed sphere where the original JEFF 3.0 data was used. In this spectrum, an extra small peak appears next to the transmitted peak and the rest of the spectrum is increased slightly (see figure 5.2). This problem shows that the pulsed spheres can be very useful to quickly assess the quality of a library file.

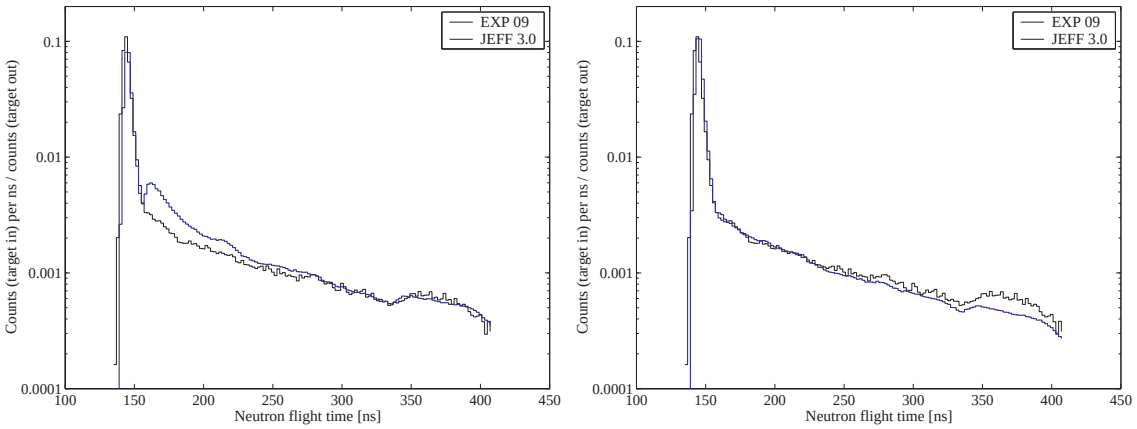

Figure 5.2: Comparison of the time of flight spectrum of a beryllium sphere using the original JEFF 3.0 evaluation where (n,2n) is counted twice (left) and the corrected evaluation (right). .

Carbon spheres

The graphs for the carbon spheres can be found in figures 5.13 to 5.18. The three types of carbon spheres (with radii of 4.187, 10.16 and 20.96 cm) are solid spheres of 99.995% carbon. These carbon spheres are very interesting examples simply because the transmitted peak, elastic, discrete inelastic and continuum inelastic regions are quite well separated. If we take for instance figure 5.17, then the spectrum between roughly 160 and 225 ns is mainly determined by the first level of inelastic scattering (4.43 MeV). The second level (7.66 MeV) determines the spectrum between 200 and 325 ns, ...
For the carbon spheres, we observe three families of curves: ENDF (being ENDF60, ENDF66, ENDF/B-VI.8, JEFF 3.0 and JEFF 3.1), JEF 2.2 (based on ENDF/B-V) and JENDL 3.3. The global agreement between the different libraries is quite good (it should be said that all libraries except for JENDL 3.3 are based on ENDF/B data). The agreement with the measured spectrum is however the best for JENDL 3.3.

Liquid nitrogen spheres

The liquid nitrogen spheres can be found in figure 5.19 and 5.20. For the nitrogen spheres, there are two configurations. Both consist of an inner sphere filled with liquid nitrogen that is placed inside another sphere. In between the spheres, there is a vacuum. The composition of the casing material is the same as the one used in the lithium spheres (except that the normal density of 7.9 g cm^{-3} is used). For the first configuration, these spheres have radii of 19.11 and 22.55 cm. For the second configuration this is 55.93 and 61.11 cm.
The best results for these liquid nitrogen spheres are obtained with JEFF 3.1 and ENDF/B-VI.8 (it should be noted that the nitrogen evaluations in JEFF 3.1 are all ENDF/B-VI evaluations).

Liquid oxygen spheres

The result of the liquid oxygen sphere (with a radius of 10.50 cm) can be found in figure 5.21. The configuration of the liquid oxygen sphere is similar to that of the liquid nitrogen sphere (the inner sphere has a radius of 10.50 cm and the outer sphere has a radius of 11.28 cm).
The agreement between the different libraries and the experimental results for the oxygen sphere is not very good (especially if we compare it with for instance the carbon spheres where

the agreement was almost perfect). This might (among other reasons) be caused by the temperature of the data used to calculate time of flight spectra (which is around 300 K while the liquid nitrogen is probably a lot colder).
We also observe some differences between the JEFF 3.1 curve and the ENDF/B-VI.8 curve while the oxygen data in JEFF 3.1 is taken from ENDF/B-VI.8. The differences between both curves are therefore related to differences in the data of the casing materials of the liquid oxygen sphere. And as we will see later on for the iron spheres (see figure 5.33 to 5.38), the iron data from JEFF 3.1 and ENDF/B-VI.8 are distinctly different. Either way, the form of the measured spectrum is reproduced to some degree.

Magnesium spheres

The results for the magnesium spheres can be found in figures 5.22 to 5.25. The three types of magnesium spheres (with radii of 8.94, 16.50 and 25.50 cm) are solid spheres of magnesium.
All the ENDF libraries and the JEFF 3.0 library are in good agreement with the measured spectrum. The JENDL 3.3 and JEFF 3.1 data on the other hand show large differences just after the transmitted peak (corresponding to neutron energies of 14 to 5 MeV). After a review of the data in question, we found that the JEFF 3.0 data (only elemental Mg) was based on JENDL 3.2 while the JENDL 3.3 data (the individual ^{24}Mg, ^{25}Mg and ^{26}Mg isotopes) were based on the same JENDL 3.2 data (with a few updates. The JEFF 3.1 data itself was simply taken over from JENDL 3.3.
As mentioned earlier, the first few levels of inelastic scattering determine the part of the time of flight spectrum just after the transmitted peak. In order to explain the differences between the spectra, we compared the data for the first levels of inelastic scattering of ^{24}Mg, ^{25}Mg and ^{26}Mg from JEFF 3.1 with those of elemental magnesium from JEFF 3.0.
The individual levels of inelastic scattering associated with ^{24}Mg, ^{25}Mg and ^{26}Mg are all different from each other and can all be found in the elemental magnesium evaluation (an overview of the corresponding levels can be found in the comment section of the ENDF file). For example, the first level of 24Mg (at 1.3686 MeV) is the third level of the elemental evaluation. The second level of ^{24}Mg (at 4.1200 MeV) is the 18th level in the elemental evaluation, ... To transform the cross section of a level from an isotope to that of the element, we need to multiply the cross section by the isotopic abundance of the isotope (78.99% for ^{24}Mg, 10.00% for ^{25}Mg and 11.01% for ^{26}Mg). The angular distributions of those inelastic levels do not need to be transformed. To transform the other cross sections (elastic, capture, ...), we need to sum the individual isotopes' cross sections multiplied by the isotopic abundances.
We found no differences in the cross sections, but we did find differences in the angular distributions of the first two levels of inelastic scattering in ^{24}Mg, (at 1.3686 and 4.1200 MeV) and ^{26}Mg (at 1.8087 and 2.9384 MeV. This can be seen in figure 5.3, which gives the first three levels of inelastic scattering of ^{24}Mg compared to the corresponding levels in the elemental magnesium data. Apart from these differences, no other major differences were found in other cross sections that can be important for the time of flight spectrum (such as elastic scattering, capture, (n,2n), ...). The difference in the spectra is probably only caused by the difference of a few angular distributions. This example alone demonstrates the power of the pulsed sphere as a simple validation benchmark.

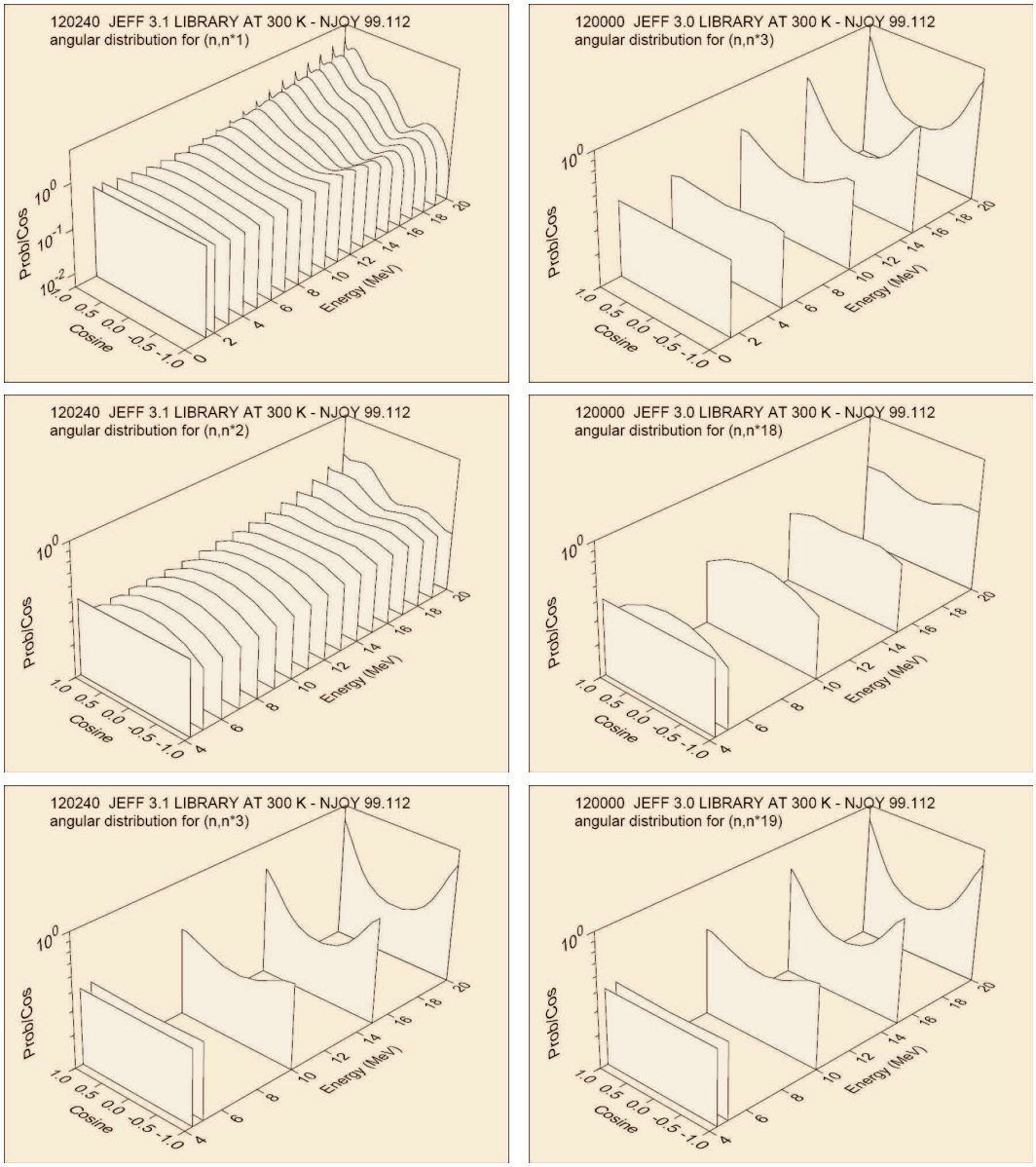

Figure 5.3: Comparison of the angular distributions of the first three inelastic scattering levels of ^{24}Mg from JEFF 3.1 (at 1.3686, 4.1200 and 4.2384 MeV) compared to the corresponding levels of elemental Mg from JEFF 3.0.

Aluminium spheres

The results for the aluminium spheres can be found in figures 5.26 to 5.29. There were three different solid aluminium spheres available (with radii of 8.94, 16.50 and 25.50 cm). The configuration of these spheres is exactly the same as those of the solid magnesium spheres.
The different nuclear data libraries give similar results below 250 ns. Above this value, the different libraries appear to have two tendencies (the first corresponding with ENDF60 and JEF 2.2 and the second with all the others). The ENDF60 and JEF 2.2 libraries give the best agreement with the experimental results. It should be noted that aluminum from ENDF/B-VI is used in JEFF 3.0 and JEFF 3.1.

Titanium spheres

The results for the titanium spheres can be found in figures 5.30 to 5.32. There were three different solid titanium spheres available (with radii of 8.94, 16.50 and 25.50 cm). The configuration of these spheres is exactly the same as those of the solid magnesium spheres.
Contrary to the results for magnesium and aluminium where all libraries (or sets of libraries) gave similar or identical results, all libraries (except the different ENDF libraries) give different results. Furthermore, none of these come even close to the experimental results. A thorough review of the titanium data relevant for these benchmarks is therefore required.

Iron spheres

The results for the iron spheres can be found in figures 5.33 to 5.38. There were three different solid iron spheres available (with radii of 4.46, 13.41 and 22.3 cm).
Except for the older JEF 2.2 evaluations of iron, all libraries appear to give good agreement with the measurements. We can also see that the curves obtained for ENDF libraries are higher than the ones obtained from JEFF 3.1 and JENDL 3.3 just after the transmitted peak. This supports our conclusion that the differences in the liquid oxygen sphere (see figure 5.21) are related to differences in data for the casing materials (the oxygen data in JEFF 3.1 and ENDF/B-VI.8 are the same). For those curves, the ENDF data also gave a curve above the one from JEFF 3.1 in the area just beyond the transmitted peak.
In general we can say that the JEFF 3.1 are slightly better than the ENDF/B-VI.8 evaluations, but the difference is only minor.

Lead spheres

The LLNL pulsed sphere experiments included a single lead sphere with a radius of 8.97 cm which includes a thin steel cladding (the configuration of this sphere is the same as the smallest lithium spheres). The results for this sphere can be found in figure 5.39.
For this lead sphere, we see a good agreement of all the libraries with the experimental results (except maybe for JEF 2.2 between 175 and 250 ns). The JEF 2.2 data is the oldest (which is a revised ENDF/B-IV evaluation). In the ENDF data we find an older ENDF/B-VI evaluation with an upper energy of 20 MeV (ENDF60) and a newer evaluation with an upper energy of 150 MeV (ENDF66 and ENDF/B-VI.8). The JEFF 3.1 evaluations are new evaluations prepared by NRG (The Netherlands) in 2004. Although the evaluations are quite different, we can see that all libraries appear to give rather similar results.

Light and heavy water spheres

The water spheres (both normal light water and heavy water) are similar to the liquid oxygen and nitrogen spheres in configuration. The results for these spheres can be found in figures 5.41 to 5.43 for the light water spheres and 5.44 to 5.45 for the heavy water spheres.
For both light water and heavy water, the different libraries give almost the same results. The neutron scattering in these spheres is primarily dominated by scattering interaction with hydrogen and deuterium. The other nuclides in these spheres like oxygen or iron are not as important. Most library families contain different evaluations for hydrogen and deuterium but they only differ by more than a few % and such differences cannot be discerned easily in the results.

Polyethylene spheres

Figure 5.46 to 5.48 gives the results for the solid polyethylene spheres (spheres with radii of 16.5, 25.5 and 40.4 cm). As we know from the carbon and water spheres, the different carbon and hydrogen evaluations give very similar results so that it does not come as a surprise that the results for polyethylene are also very similar.
It is even possible to discern the influence of the carbon data. The small peaks that appear at 175 ns and 200 ns are probably caused by the first and second inelastic scattering levels, as we observed for the carbon spheres (although the effects of these inelastic levels was more pronounced in those cases).
We also saw that the carbon data results in three different families of curves in the carbon spheres (ENDF, JEF 2.2 and JENDL). In this case, we cannot see these three families because the hydrogen scattering is dominant.

Teflon spheres

Figure 5.49 to 5.52 gives the results for the solid teflon spheres. Contrary to the previous polyethylene spheres, the carbon data is now dominant. And as a result, we can observe the same three families of curves from the carbon data: ENDF (being ENDF60, ENDF66, ENDF/B-VI.8, JEFF 3.0 and JEFF 3.1), JEF 2.2 and JENDL 3.3.

Concrete spheres

The concrete results can be found in figures 5.53 and 5.54. Again, these are solid spheres of concrete (55.70% O, 15.10% H, 14.90% Si, 3.60% Ca, 3.20% Al, 3.10% C, 1.80% Mg, 1.30% Na, 0.325% Fe, 0.325% K, 0.325% Ti and 0.325% Mn) with radii of 21.0 and 35.5 cm.
The agreement for the different libraries in the case of the concrete sphere is astonishing, especially when we know that there are 12 different elements in this particular instance of concrete (there are literally thousands of different possible compositions of concrete). This is however a pulsed sphere experiment that does not give much information concerning the nuclear data (simply because the number of materials involved is too high). In order to learn something from the results, the number of materials should be as small as possible. Solid spheres of a single material (such as the spheres of solid carbon, beryllium, ...) are the best way to go.

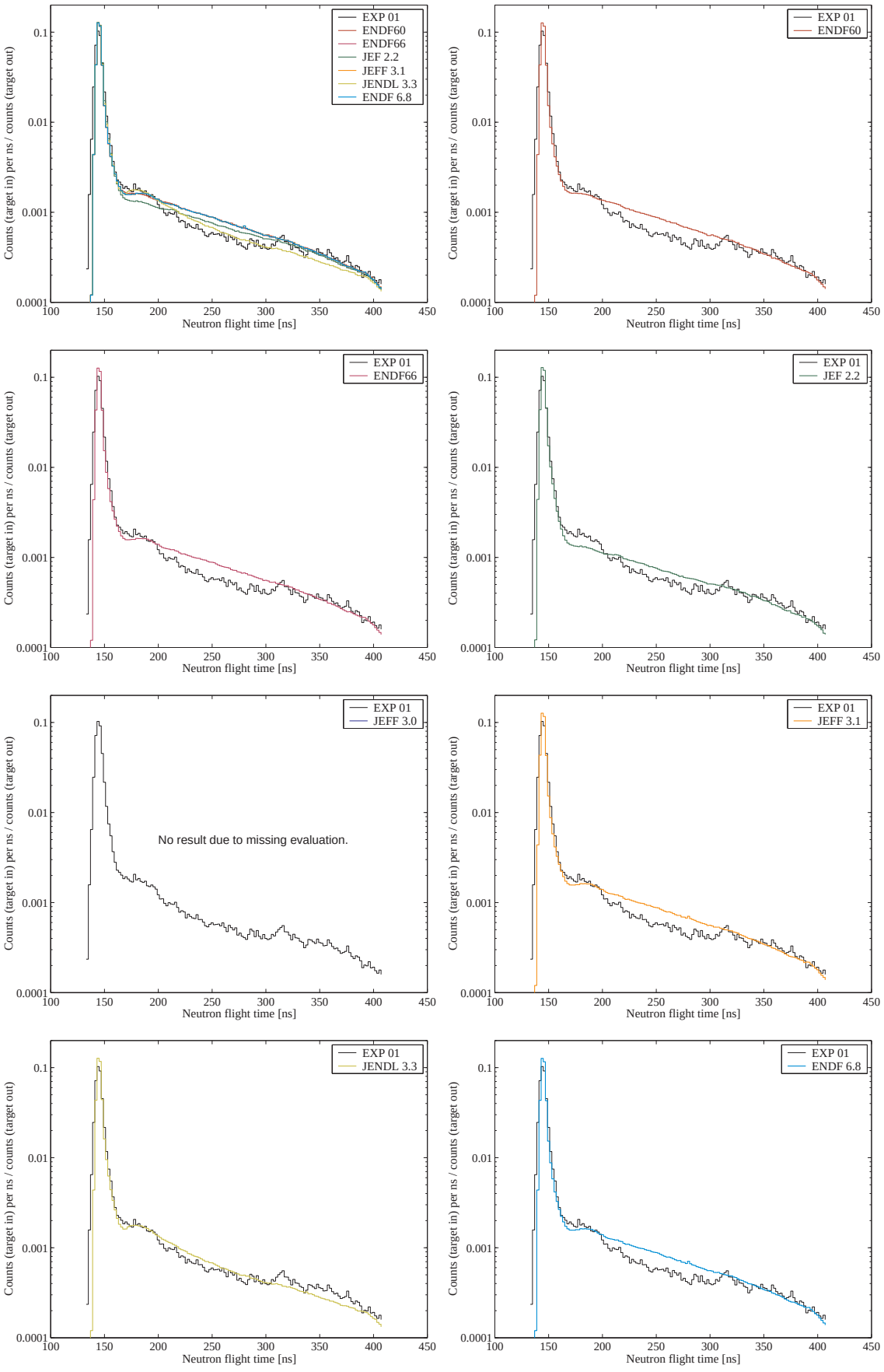

Figure 5.4: Experiment 1: ^{6}Li 0.5 mfp at 30 degrees with the Pilot B detector.

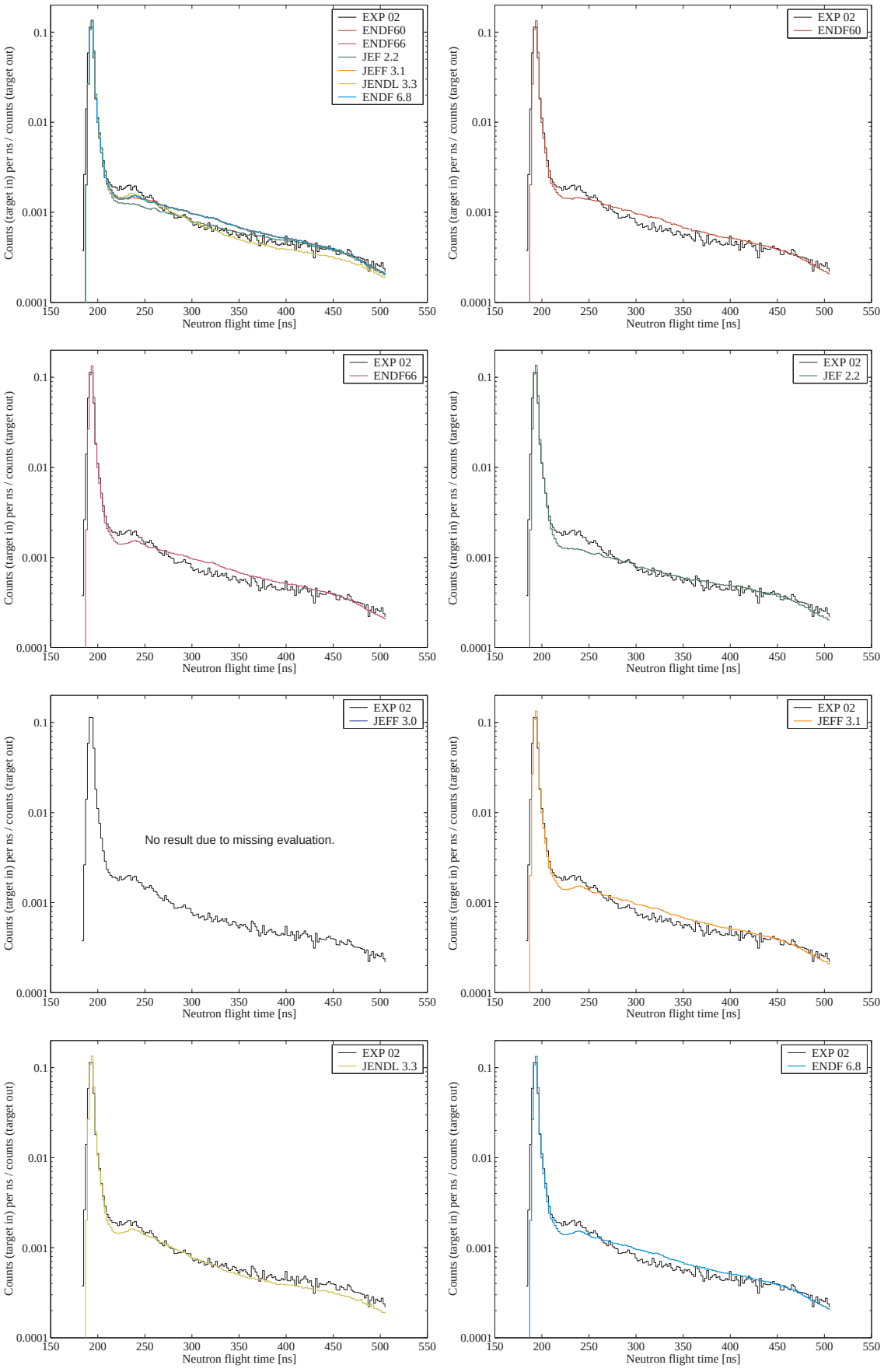

Figure 5.5: Experiment 2: ^{6}Li 0.5 mfp at 120 degrees with the NE213 detector.

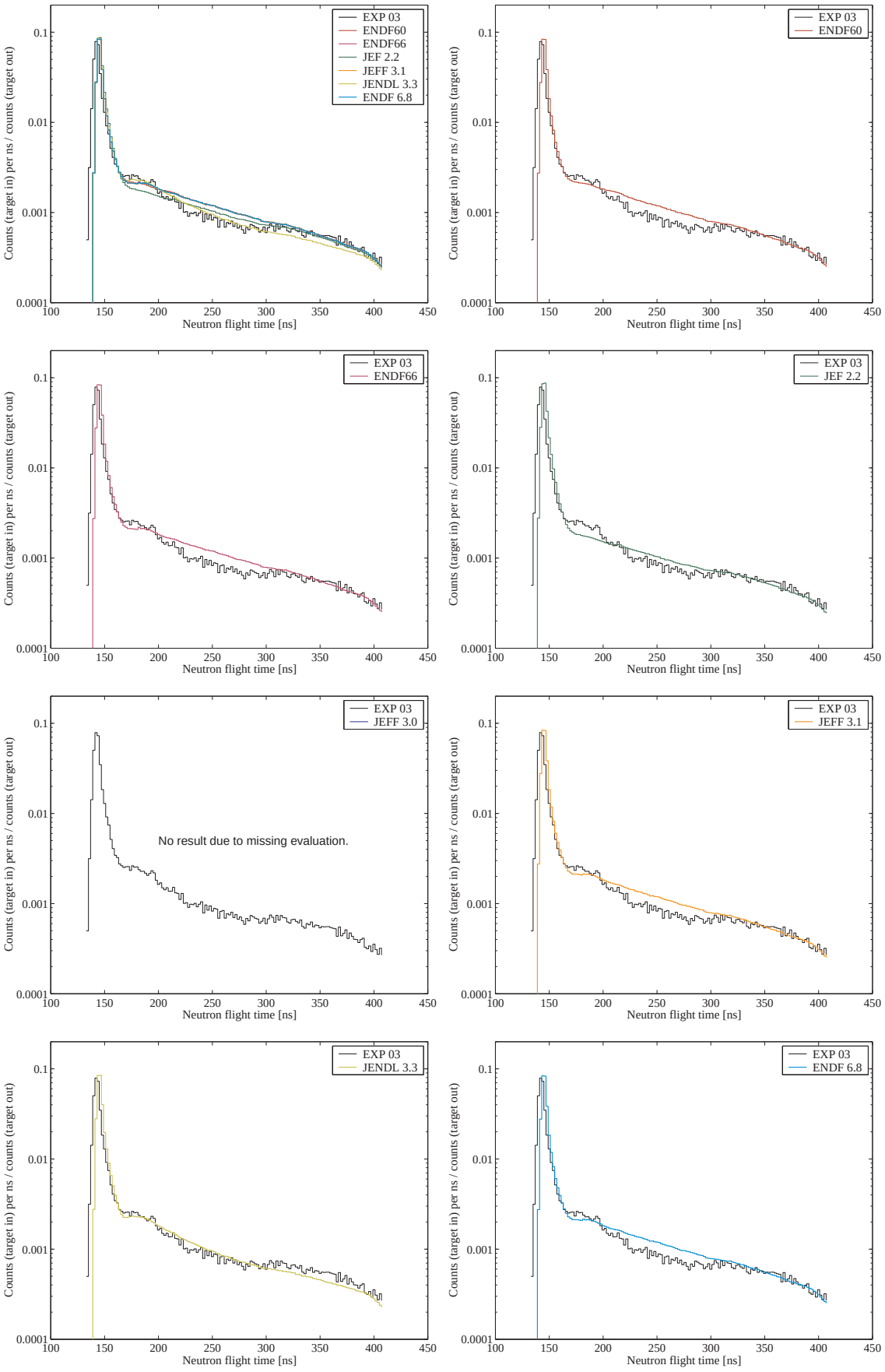

Figure 5.6: Experiment 3: ^{6}Li 1.1 mfp at 30 degrees with the Pilot B detector.

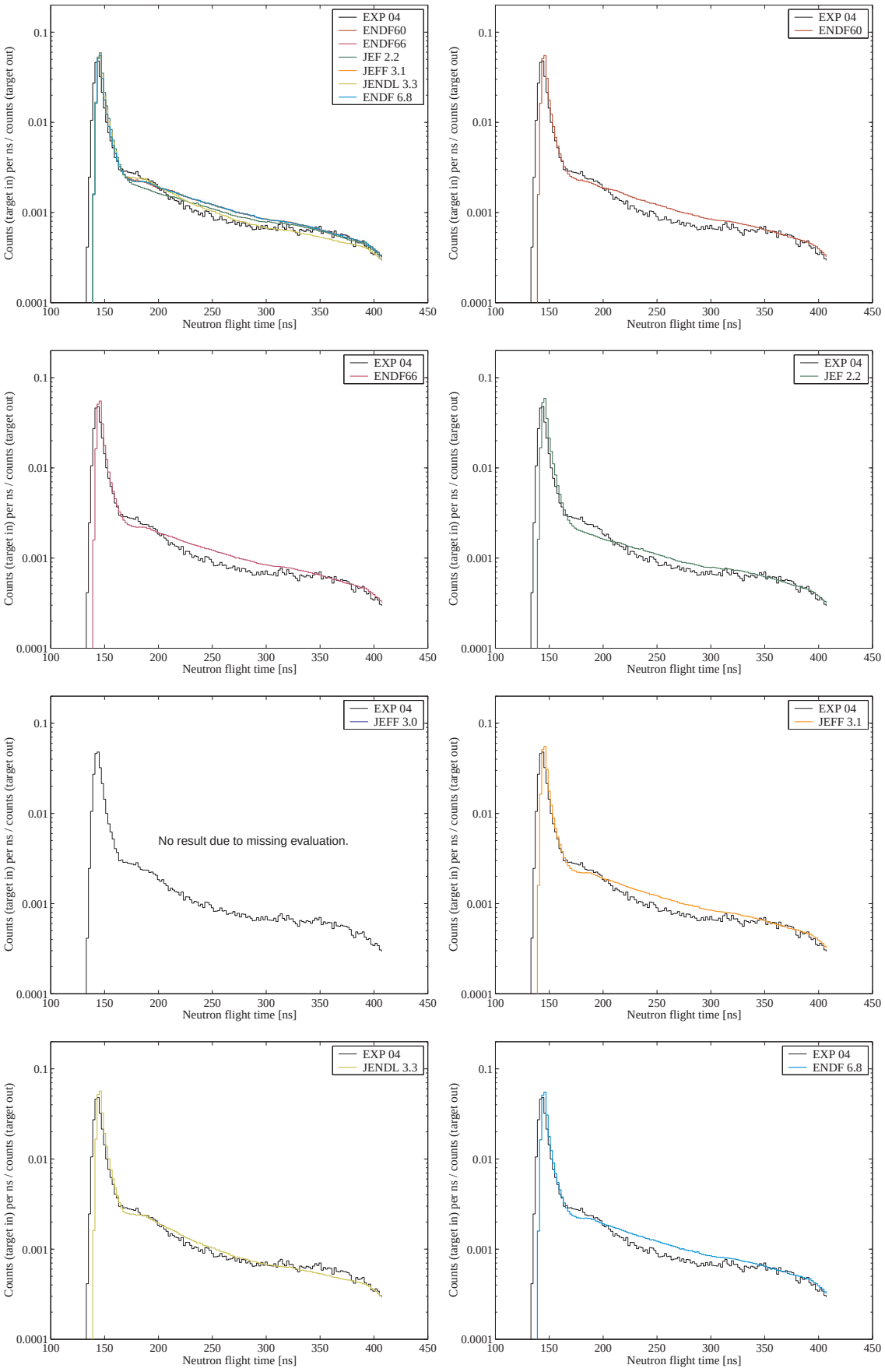

Figure 5.7: Experiment 4: ^{6}Li 1.6 mfp at 30 degrees with the Pilot B detector.

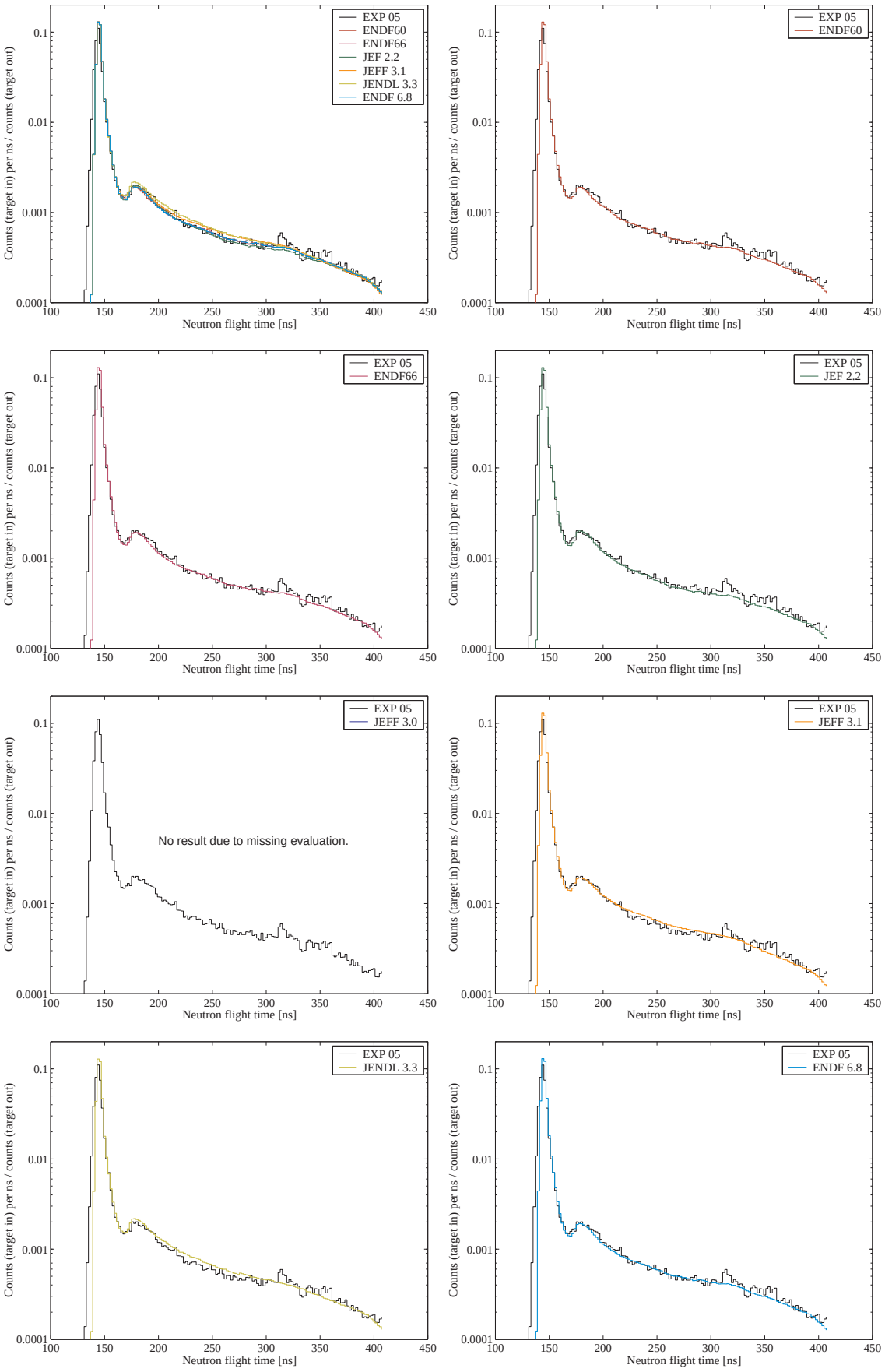

Figure 5.8: Experiment 5: ^{7}Li 0.5 mfp at 30 degrees with the Pilot B detector.

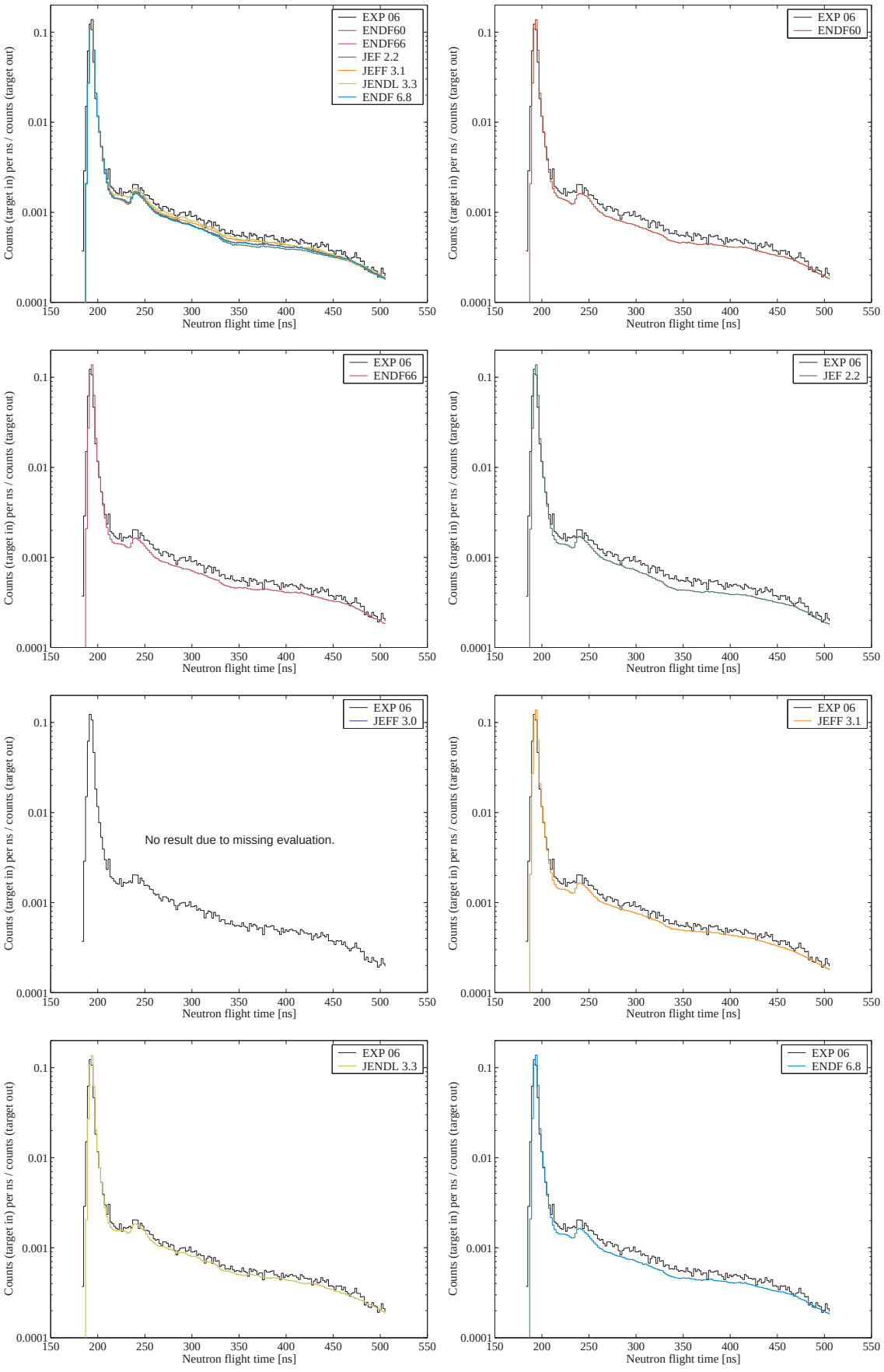

Figure 5.9: Experiment 6: ^{7}Li 0.5 mfp at 120 degrees with the NE213 detector.

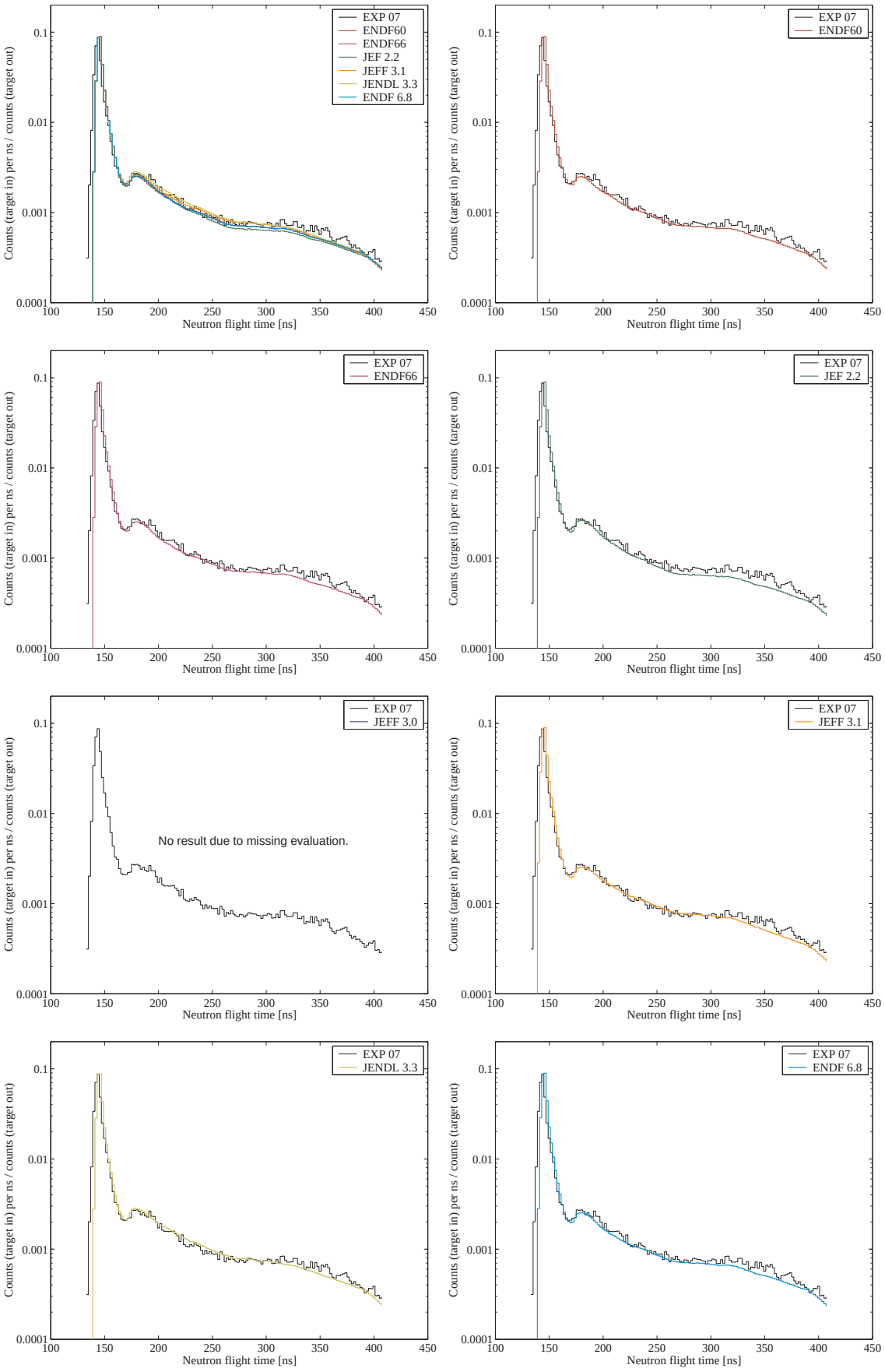

Figure 5.10: Experiment 7: ^{7}Li 1.0 mfp at 30 degrees with the Pilot B detector.

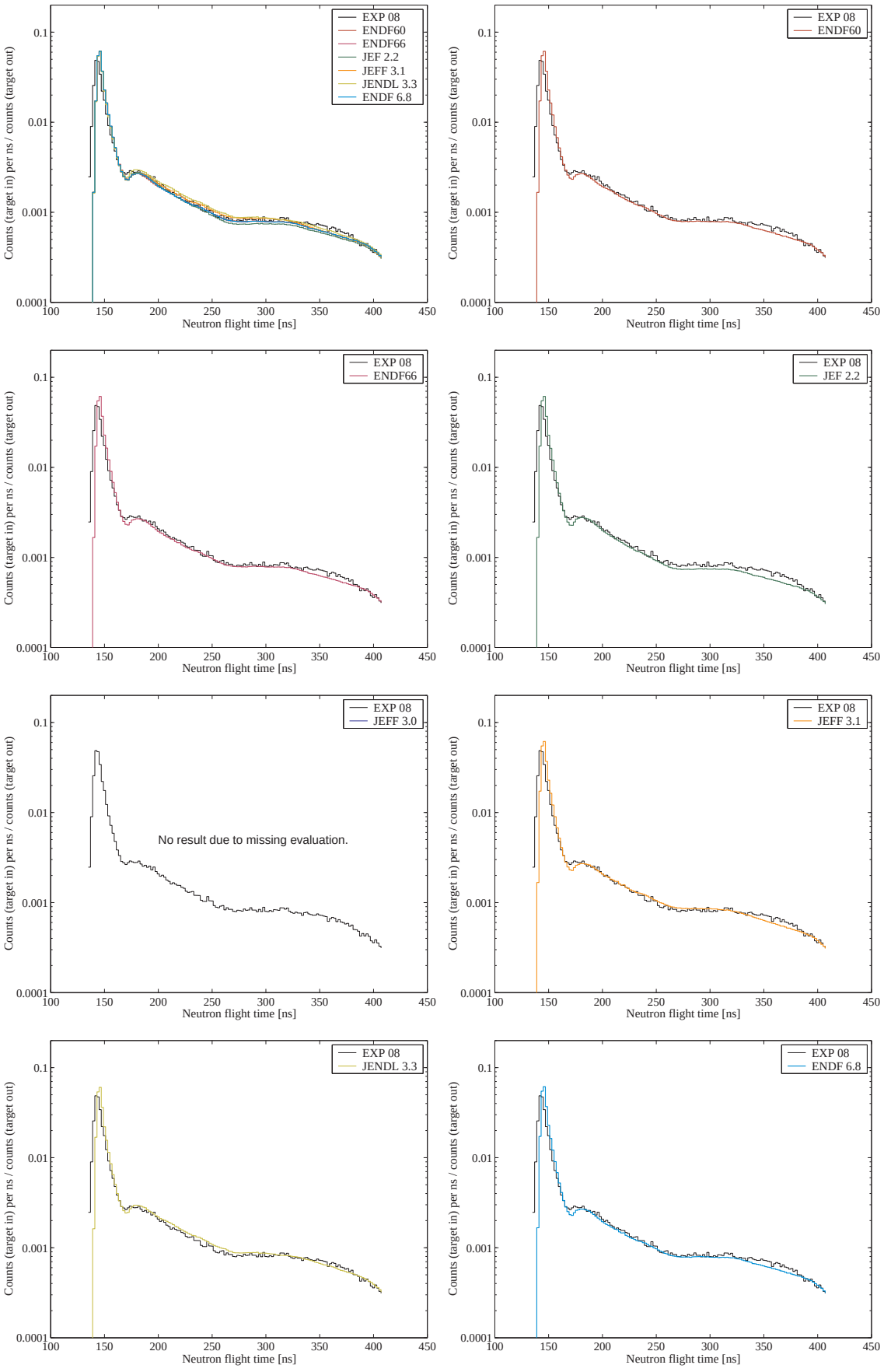

Figure 5.11: Experiment 8: ^{7}Li 1.6 mfp at 30 degrees with the Pilot B detector.

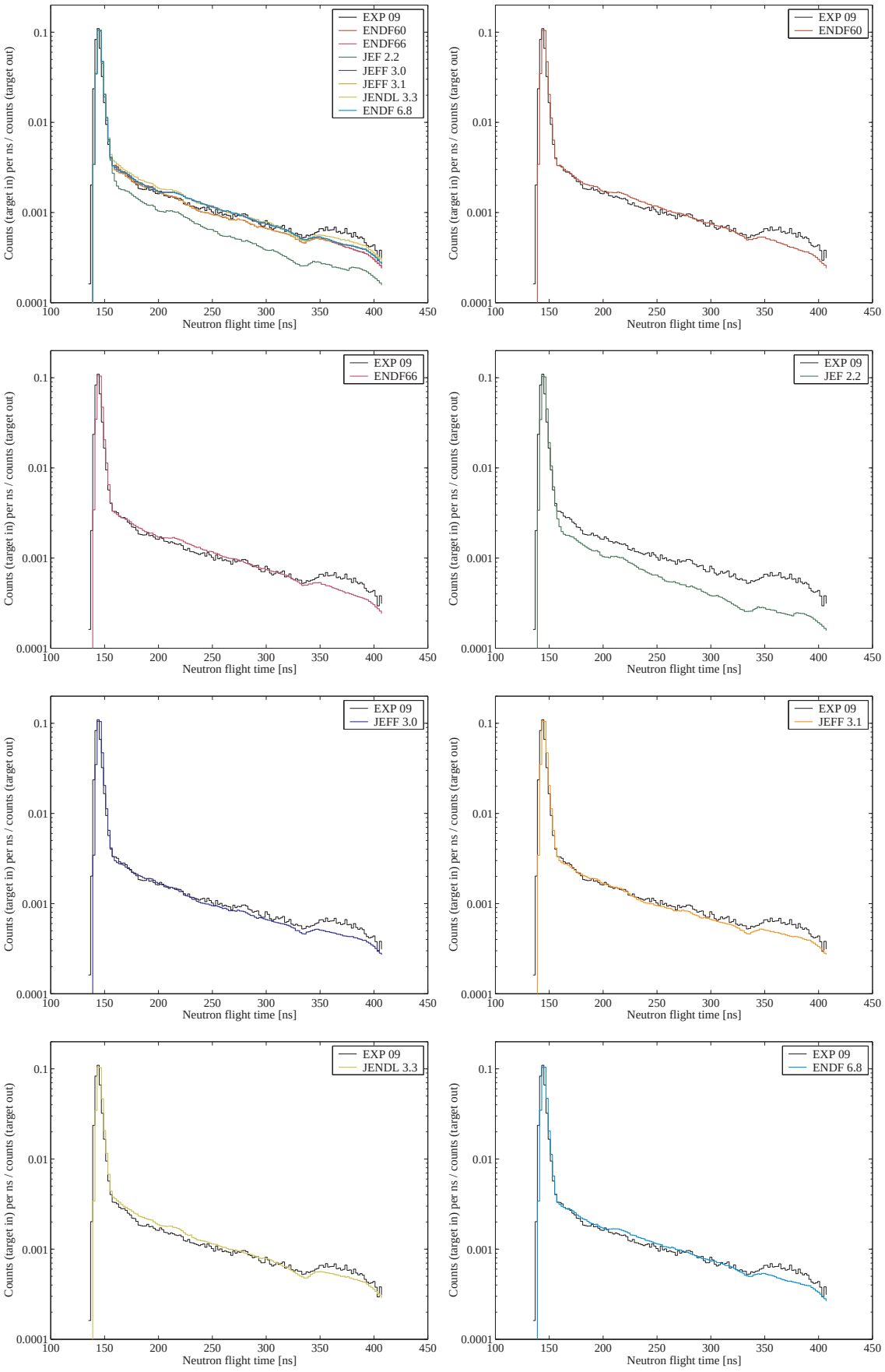

Figure 5.12: Experiment 9: Be 0.8 mfp at 30 degrees with the Pilot B detector.

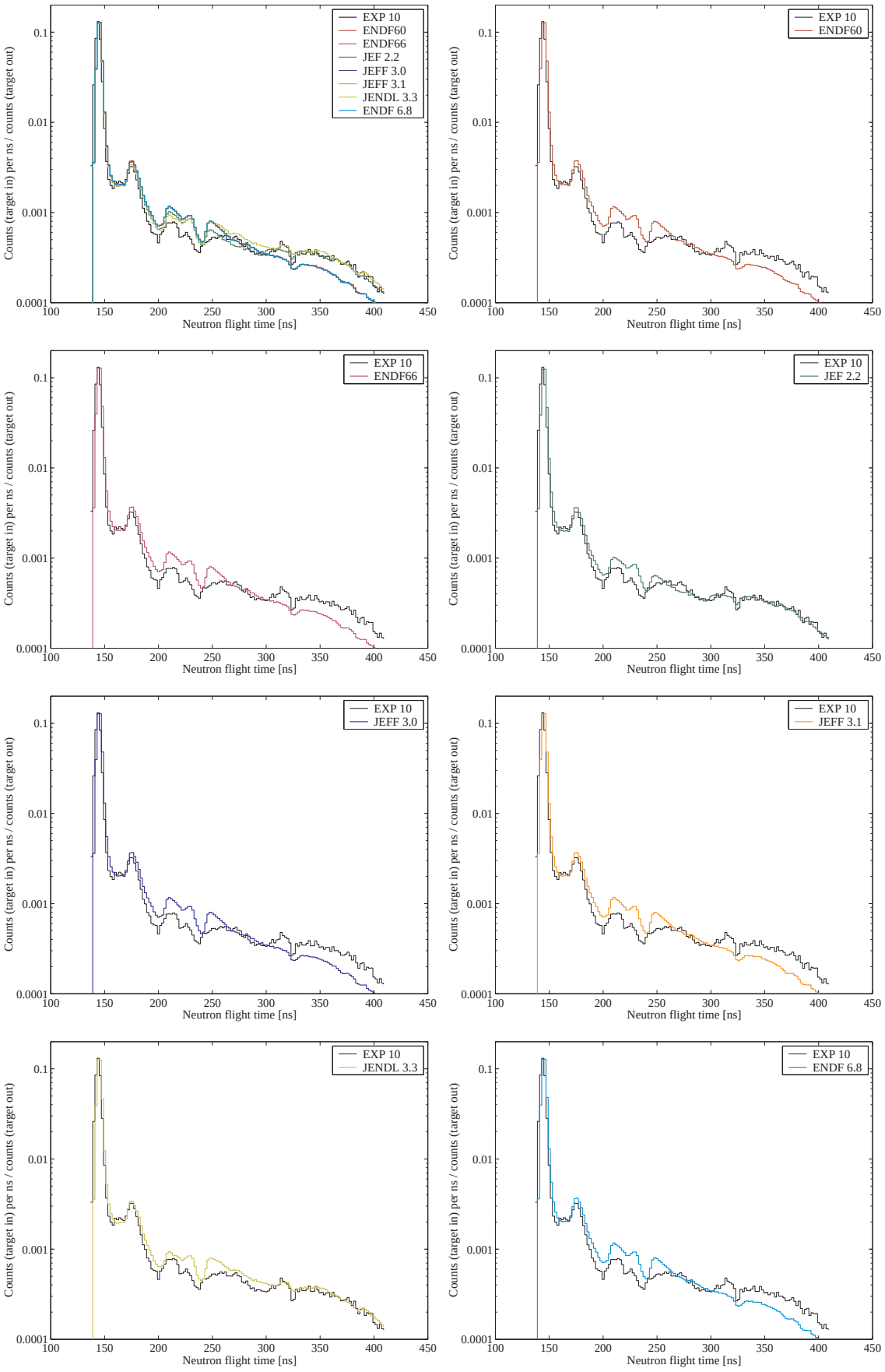

Figure 5.13: Experiment 10: C 0.5 mfp at 30 degrees with the NE213 detector.

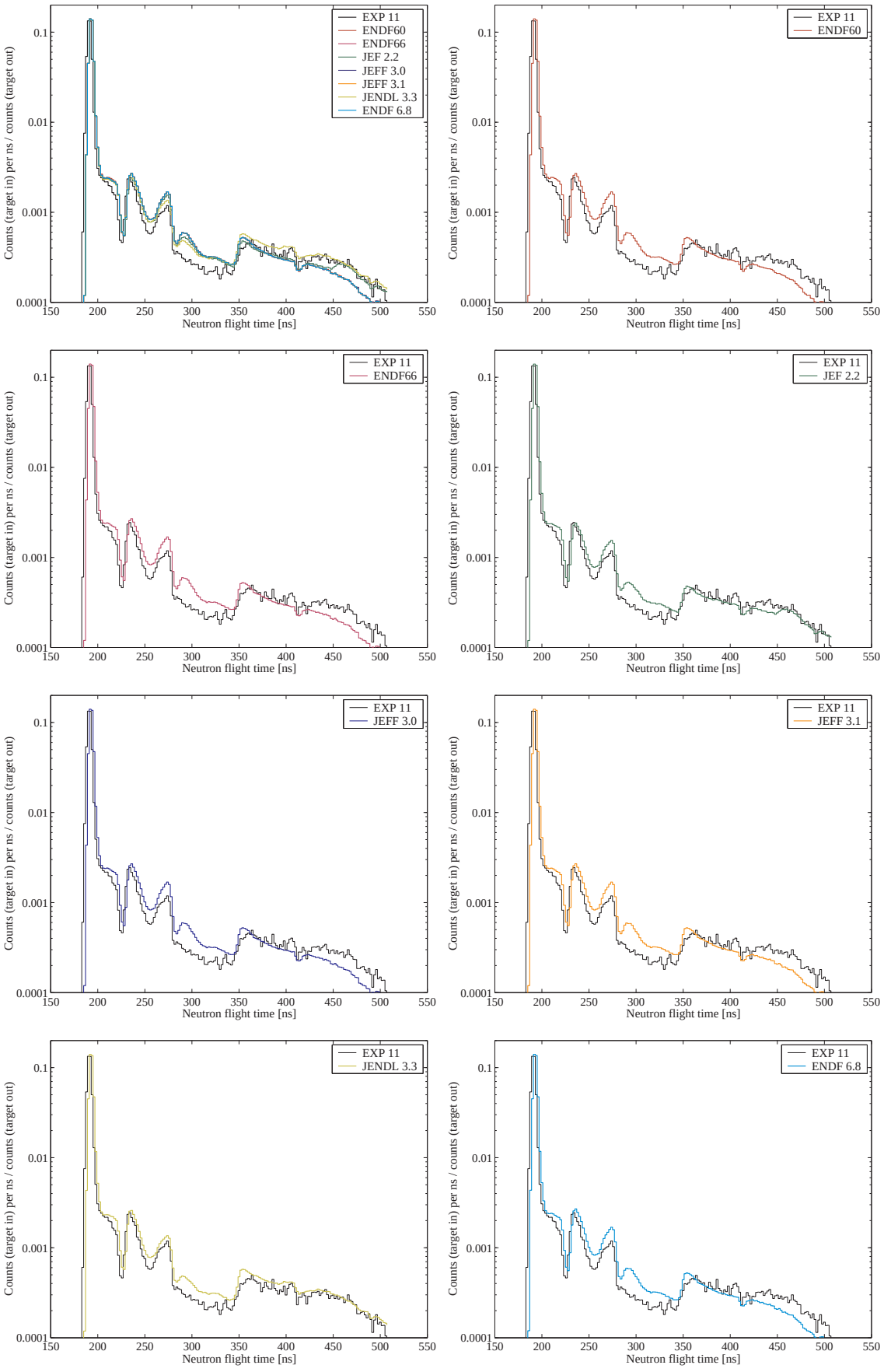

Figure 5.14: Experiment 11: C 0.5 mfp at 120 degrees with the NE213 detector.

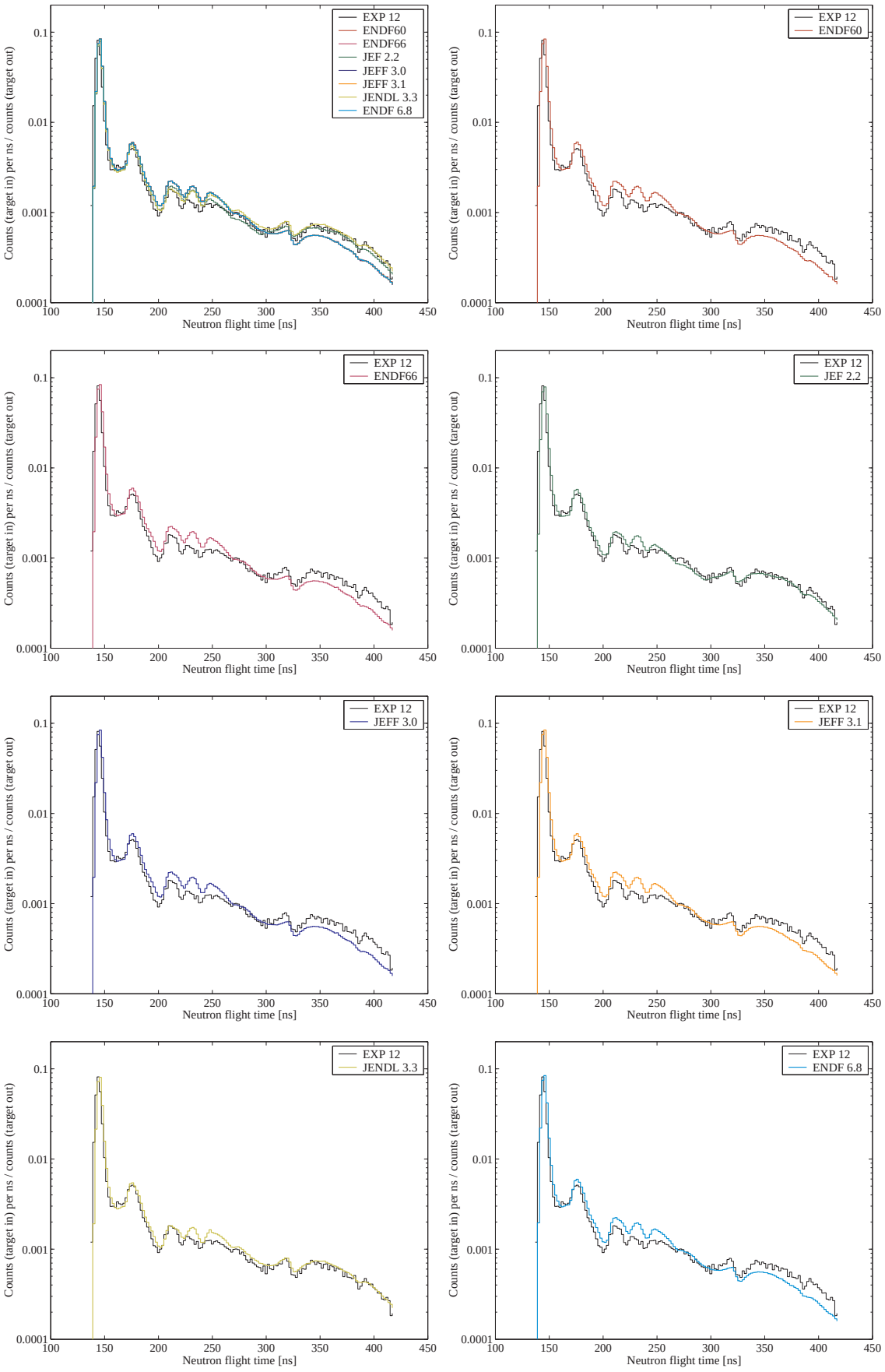

Figure 5.15: Experiment 12: C 1.3 mfp at 30 degrees with the NE213 detector.

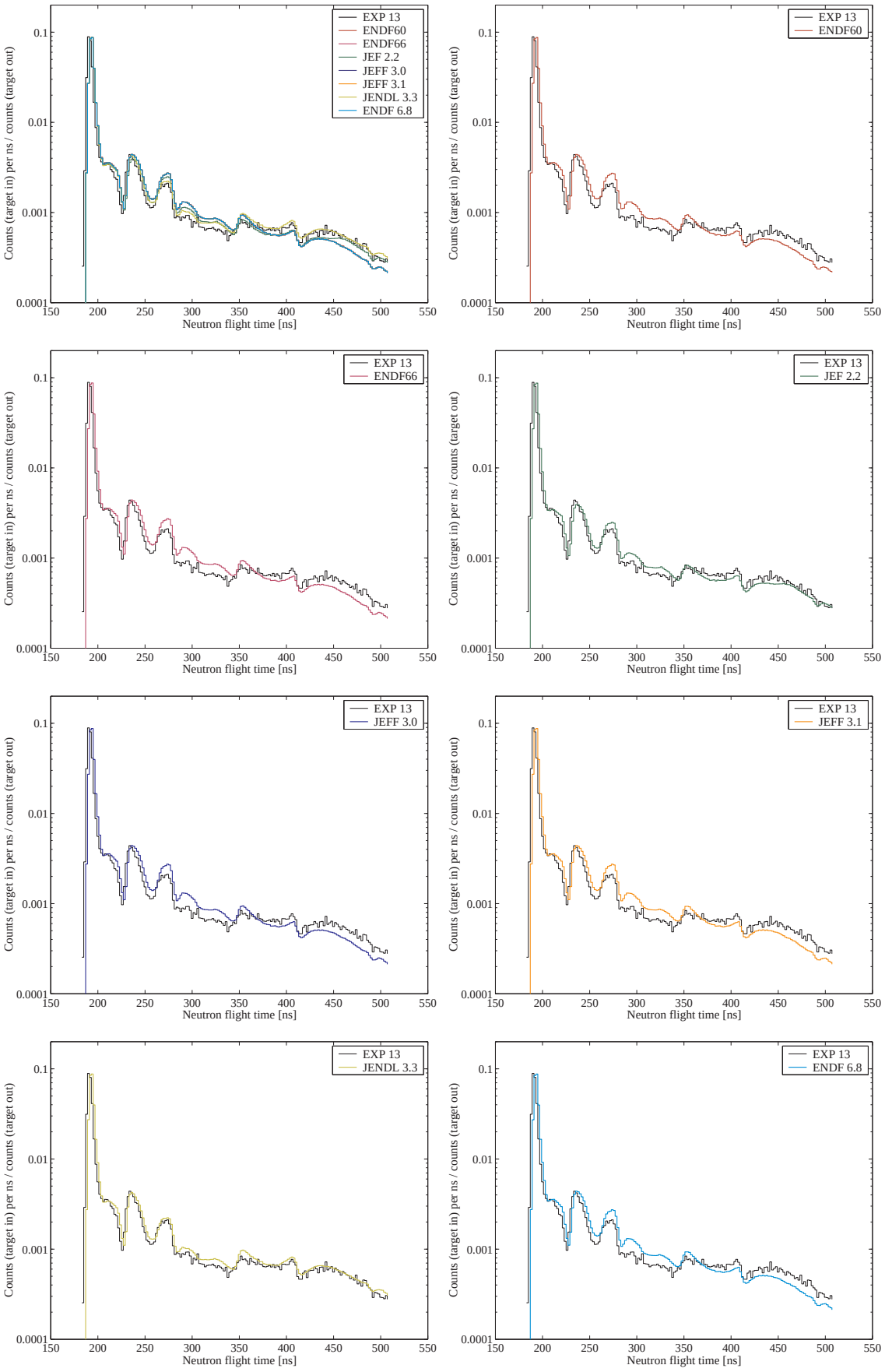

Figure 5.16: Experiment 13: C 1.3 mfp at 120 degrees with the NE213 detector.

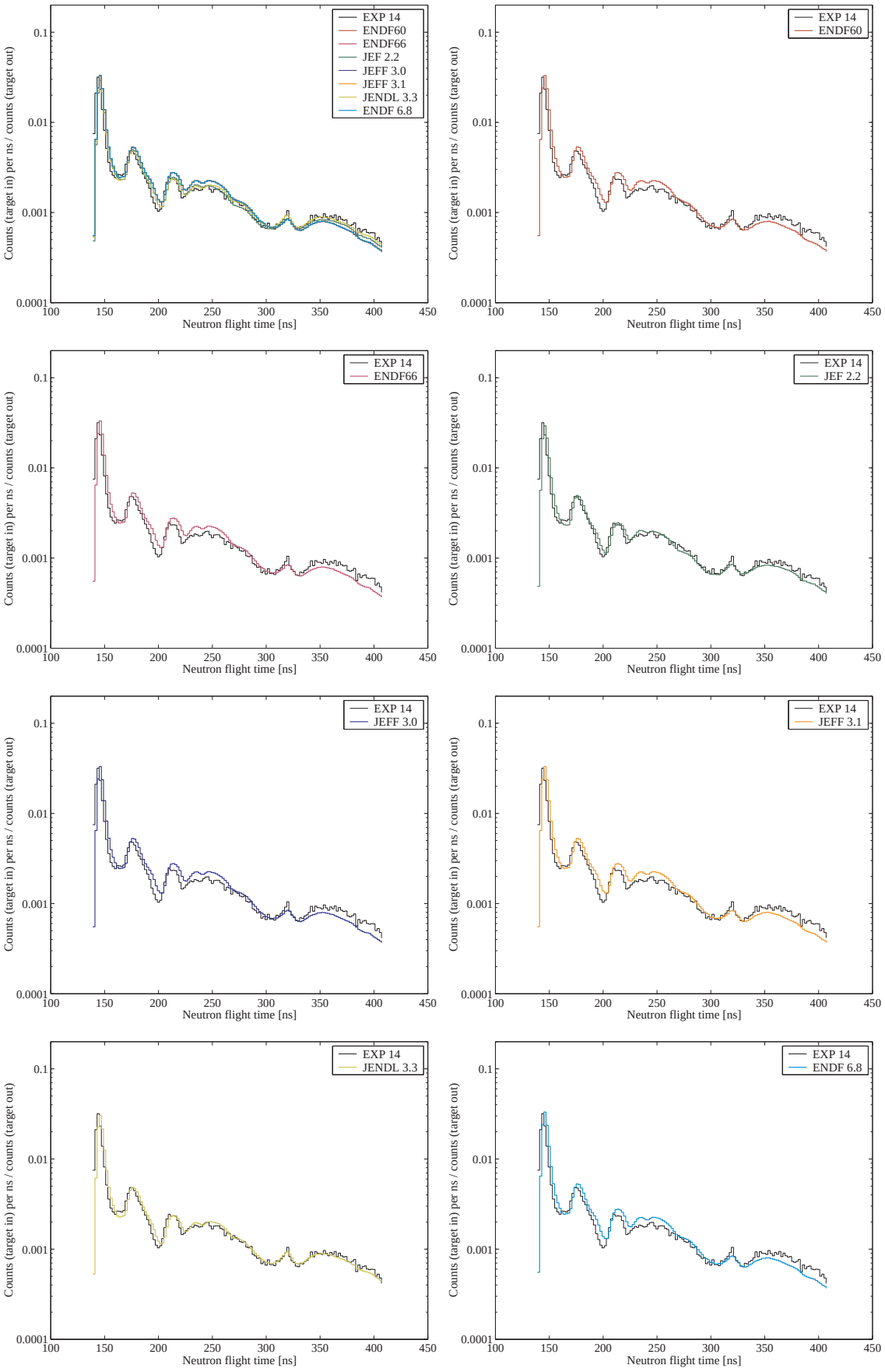

Figure 5.17: Experiment 14: C 2.9 mfp at 30 degrees with the NE213 detector.

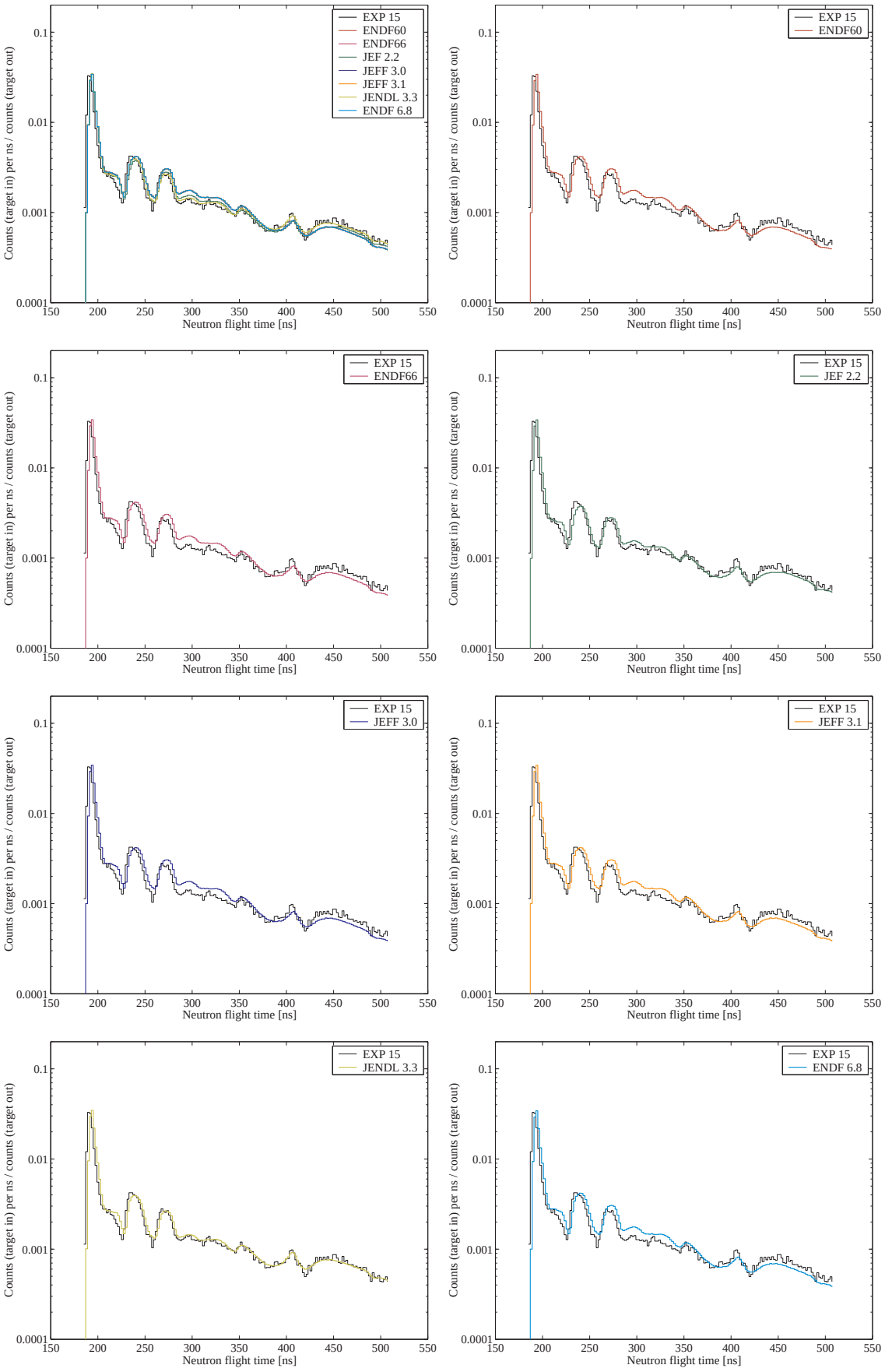

Figure 5.18: Experiment 15: C 2.9 mfp at 120 degrees with the NE213 detector.

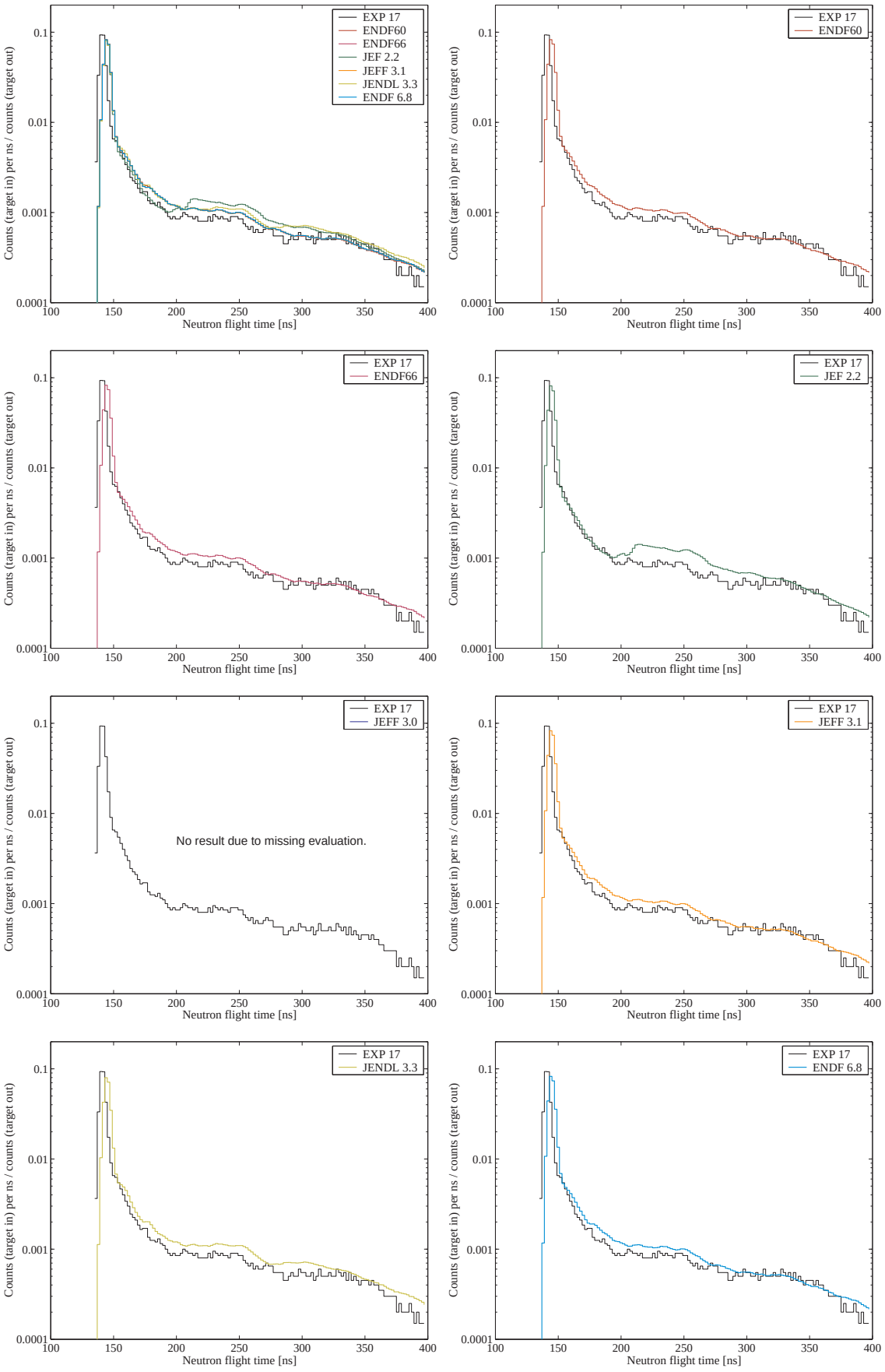

Figure 5.19: Experiment 17: N 1.1 mfp at 30 degrees with the Pilot B detector.

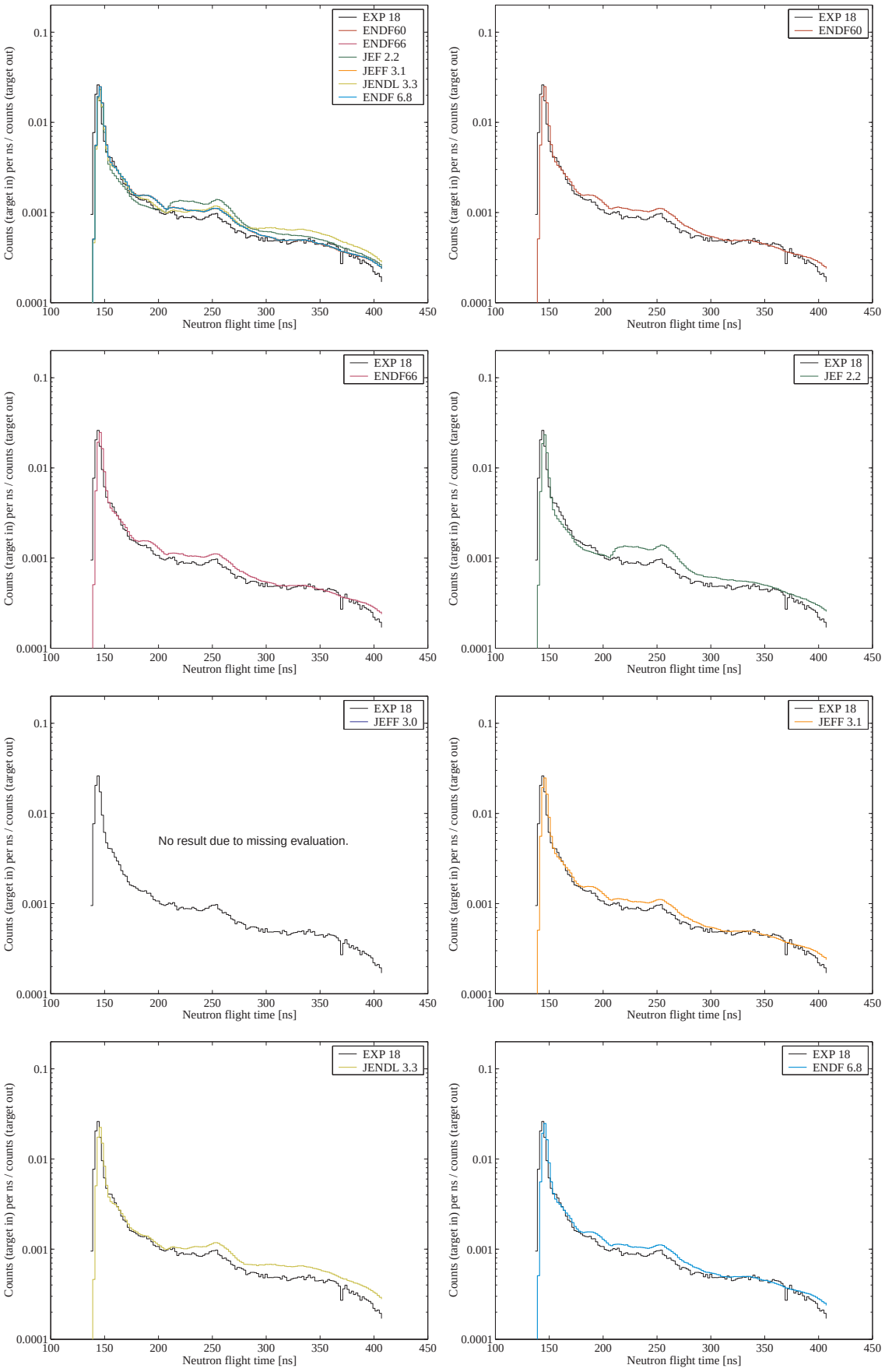

Figure 5.20: Experiment 18: N 3.1 mfp at 30 degrees with the Pilot B detector.

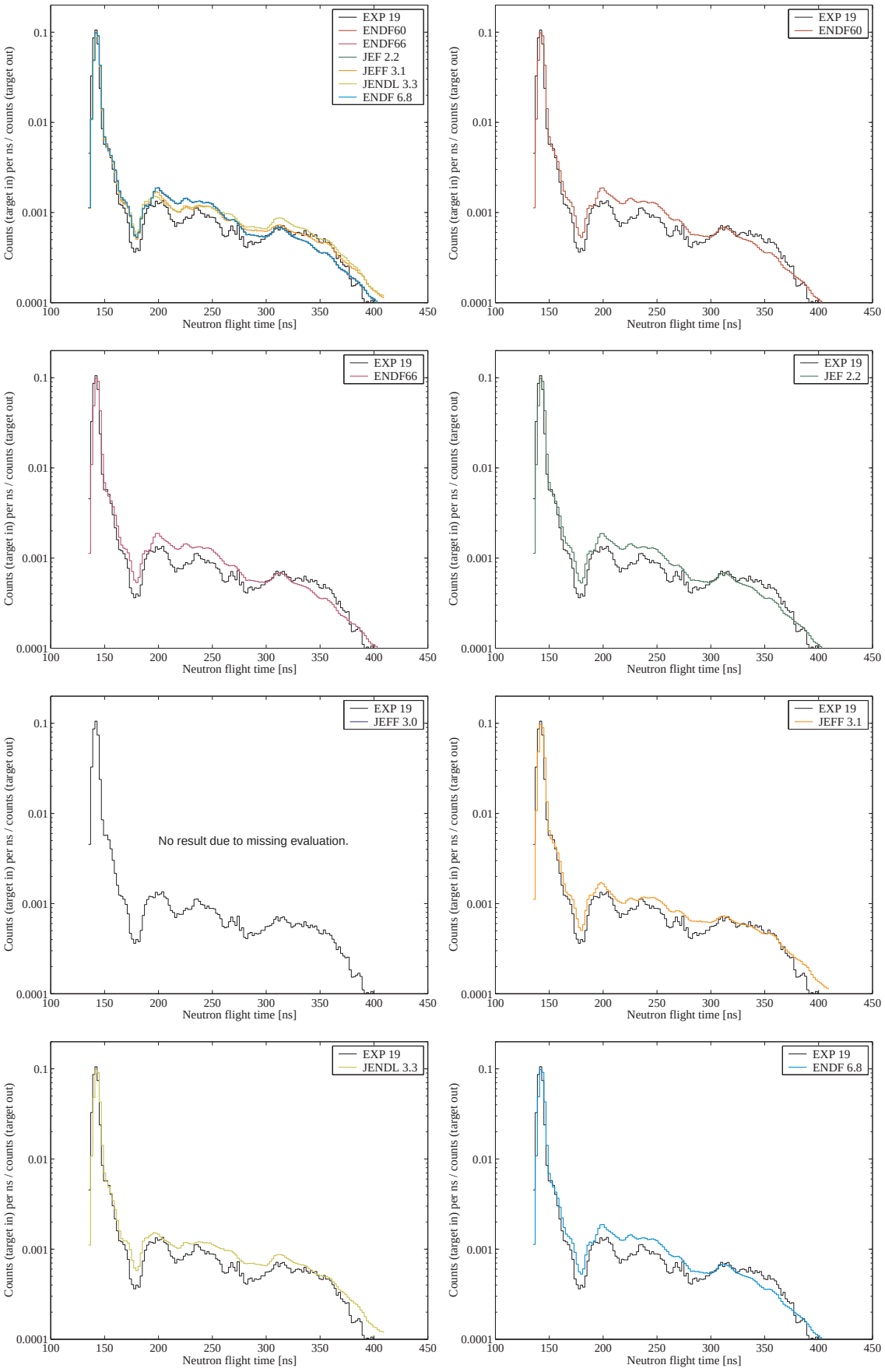

Figure 5.21: Experiment 19: O 1.1 mfp at 30 degrees with the Pilot B detector.

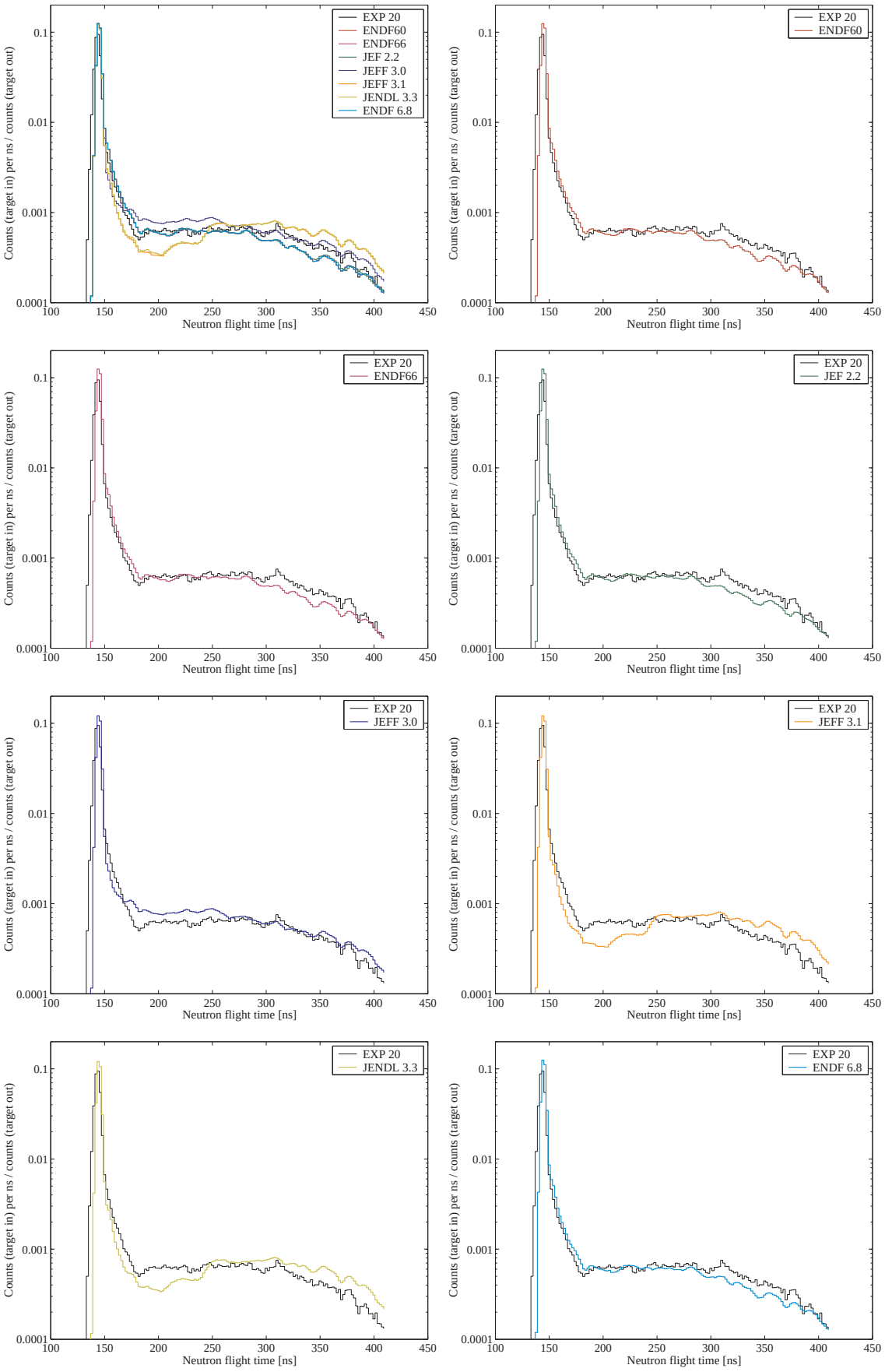

Figure 5.22: Experiment 20: Mg 0.7 mfp at 30 degrees with the Pilot B detector.

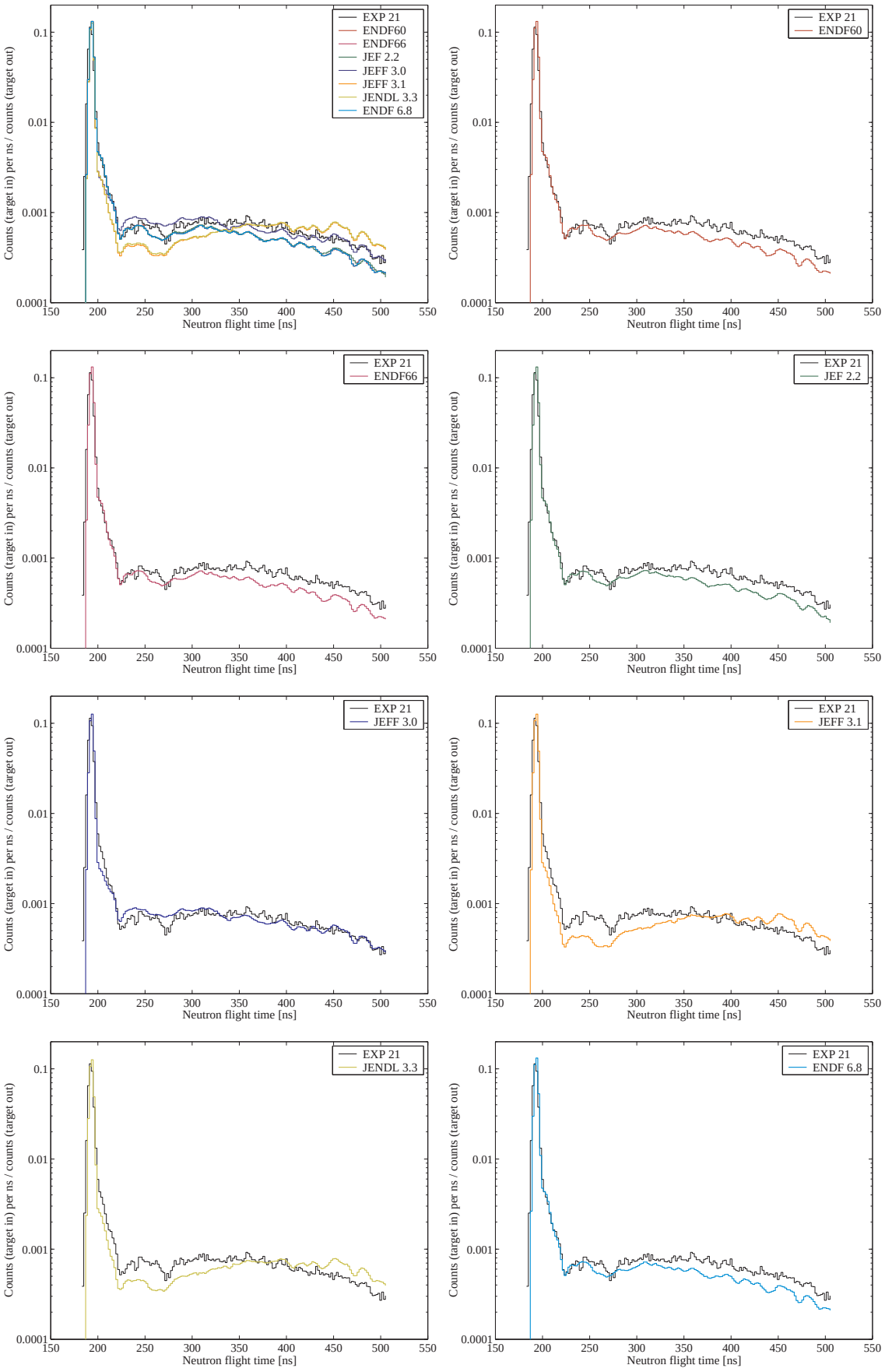

Figure 5.23: Experiment 21: Mg 0.7 mfp at 120 degrees with the NE213 detector.

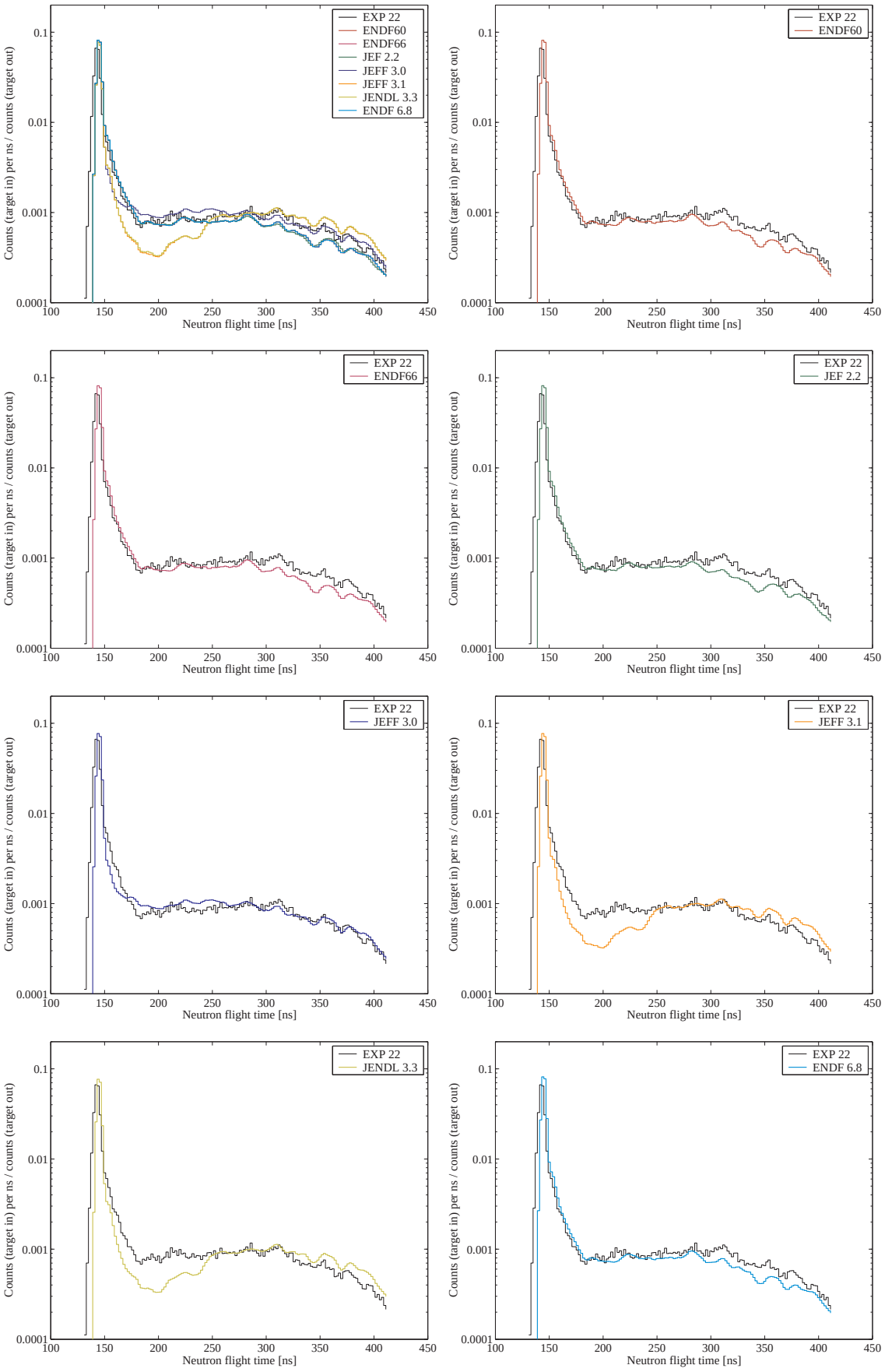

Figure 5.24: Experiment 22: Mg 1.2 mfp at 30 degrees with the Pilot B detector.

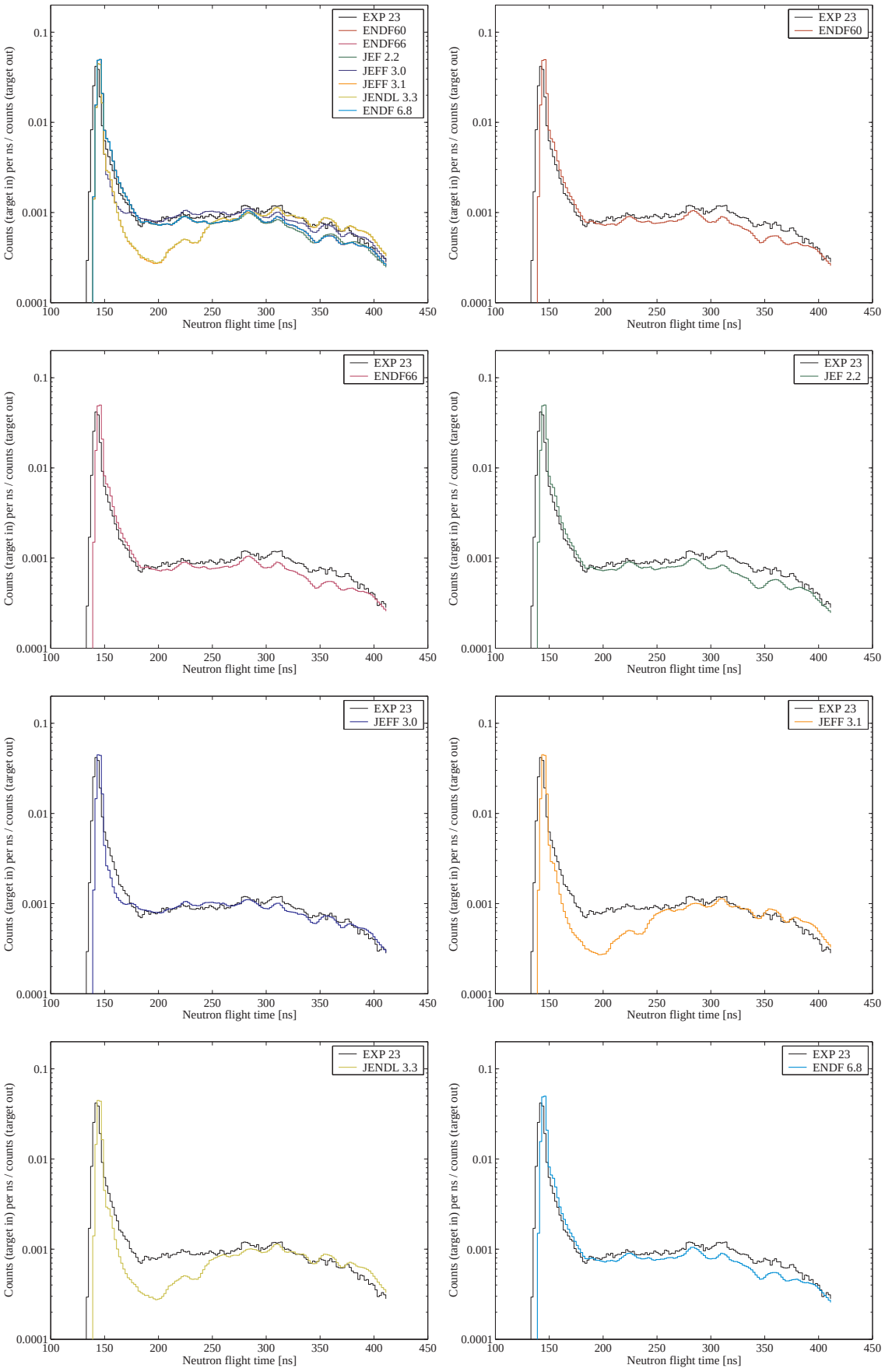

Figure 5.25: Experiment 23: Mg 1.9 mfp at 30 degrees with the Pilot B detector.

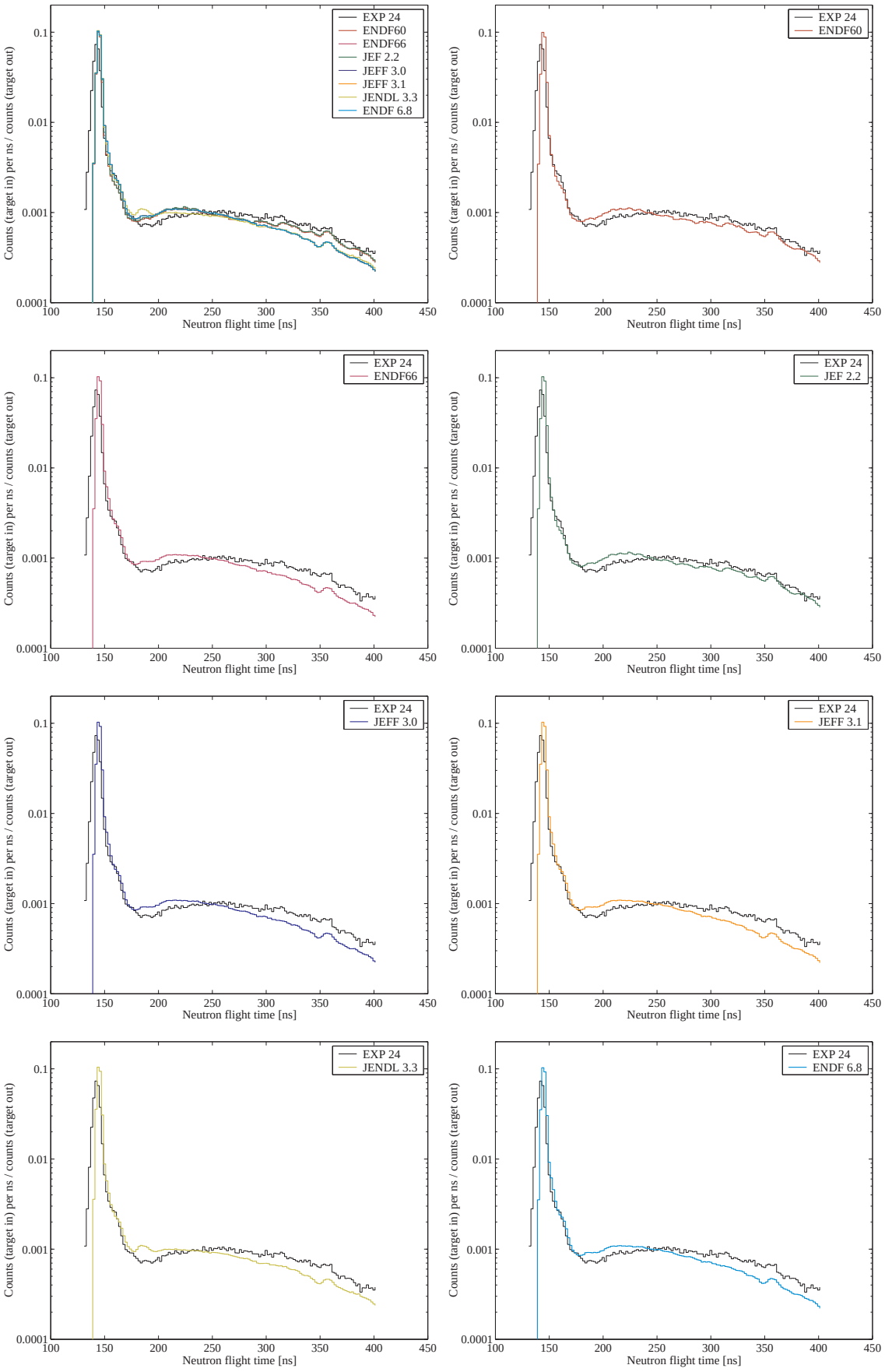

Figure 5.26: Experiment 24: Al 0.9 mfp at 30 degrees with the Pilot B detector.

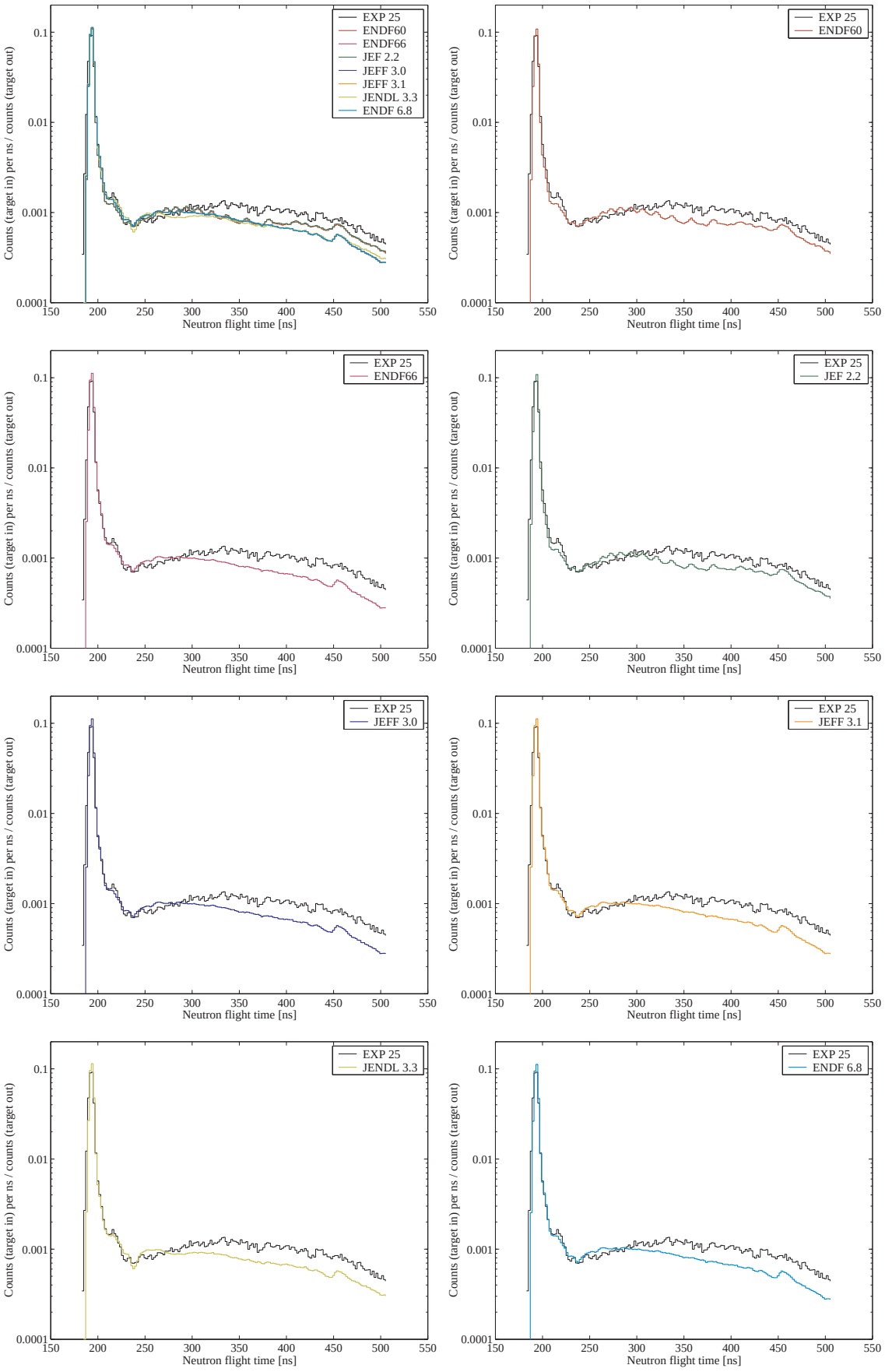

Figure 5.27: Experiment 25: Al 0.9 mfp at 120 degrees with the NE213 detector.

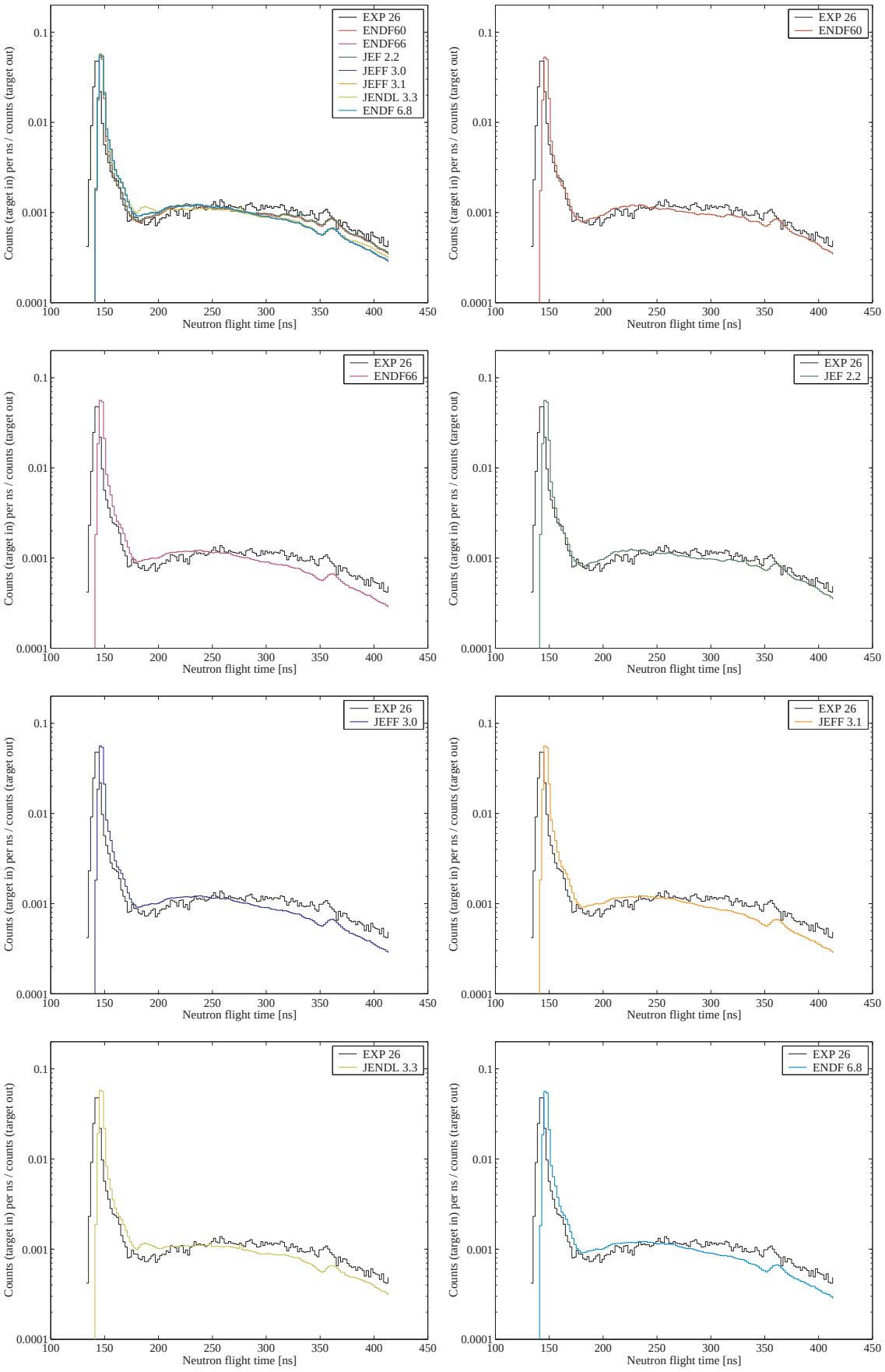

Figure 5.28: Experiment 26: Al 1.6 mfp at 30 degrees with the Pilot B detector.

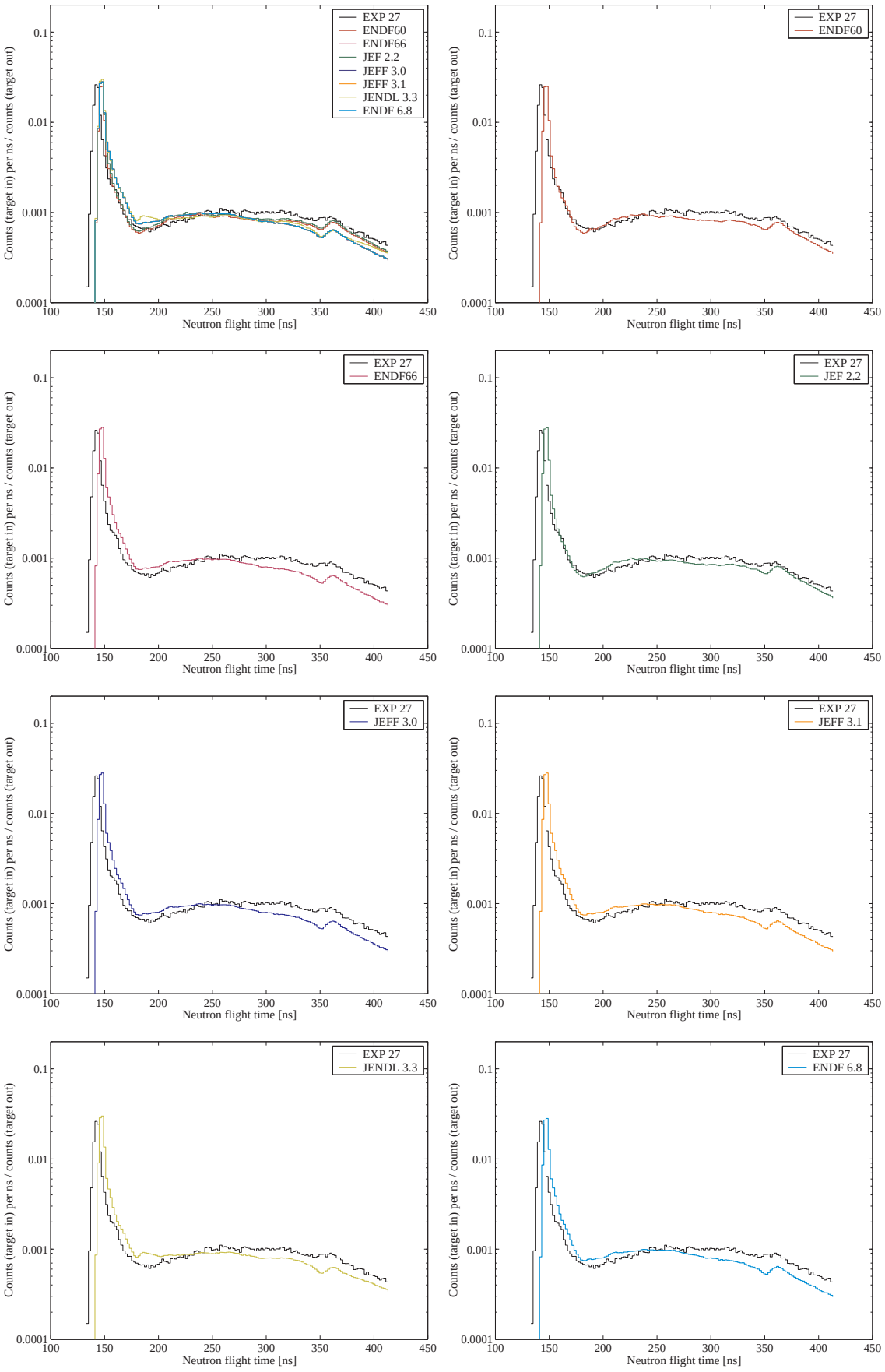

Figure 5.29: Experiment 27: Al 2.6 mfp at 30 degrees with the Pilot B detector.

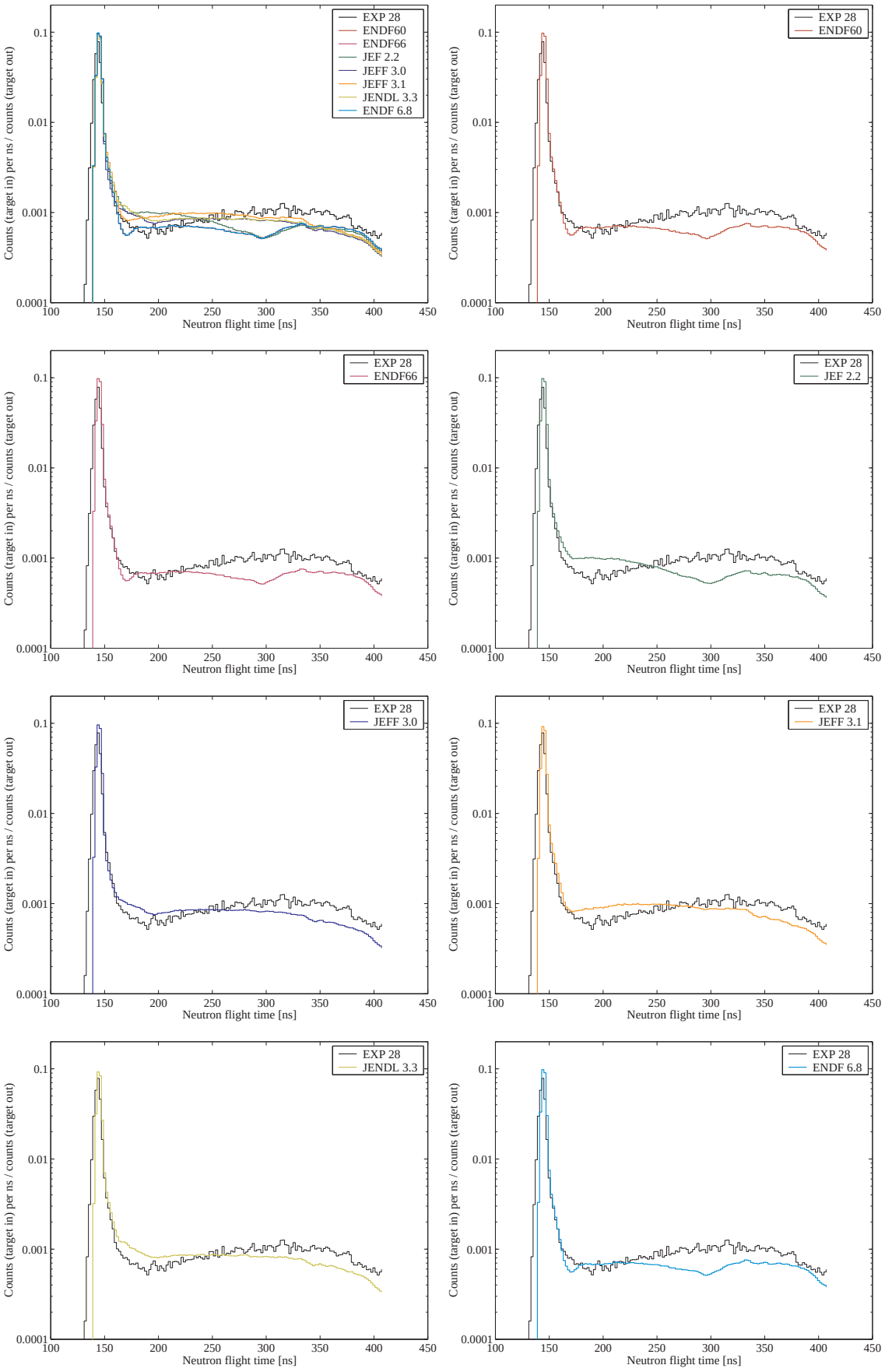

Figure 5.30: Experiment 28: Ti 1.2 mfp at 30 degrees with the Pilot B detector.

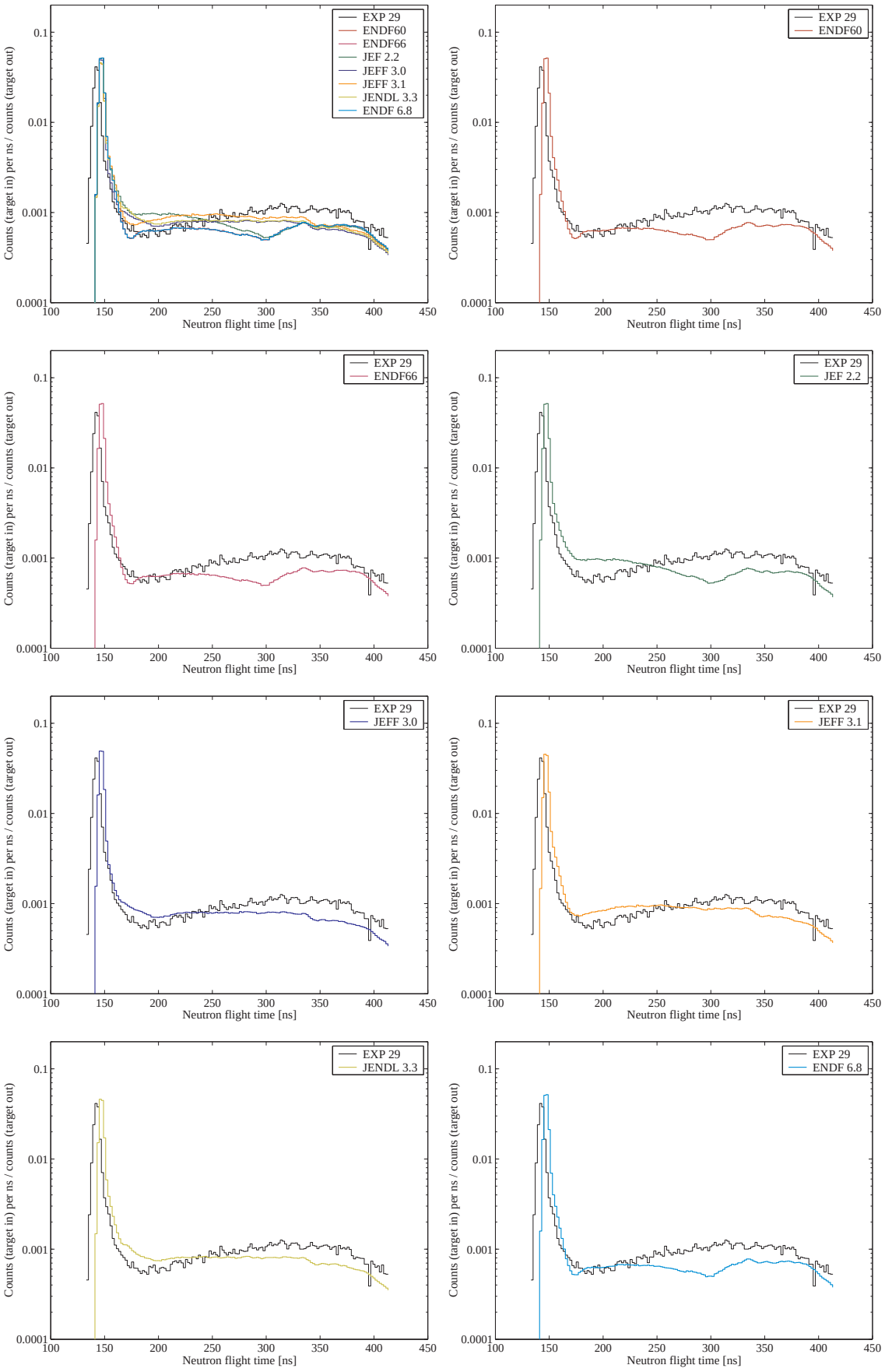

Figure 5.31: Experiment 29: Ti 2.2 mfp at 30 degrees with the Pilot B detector.

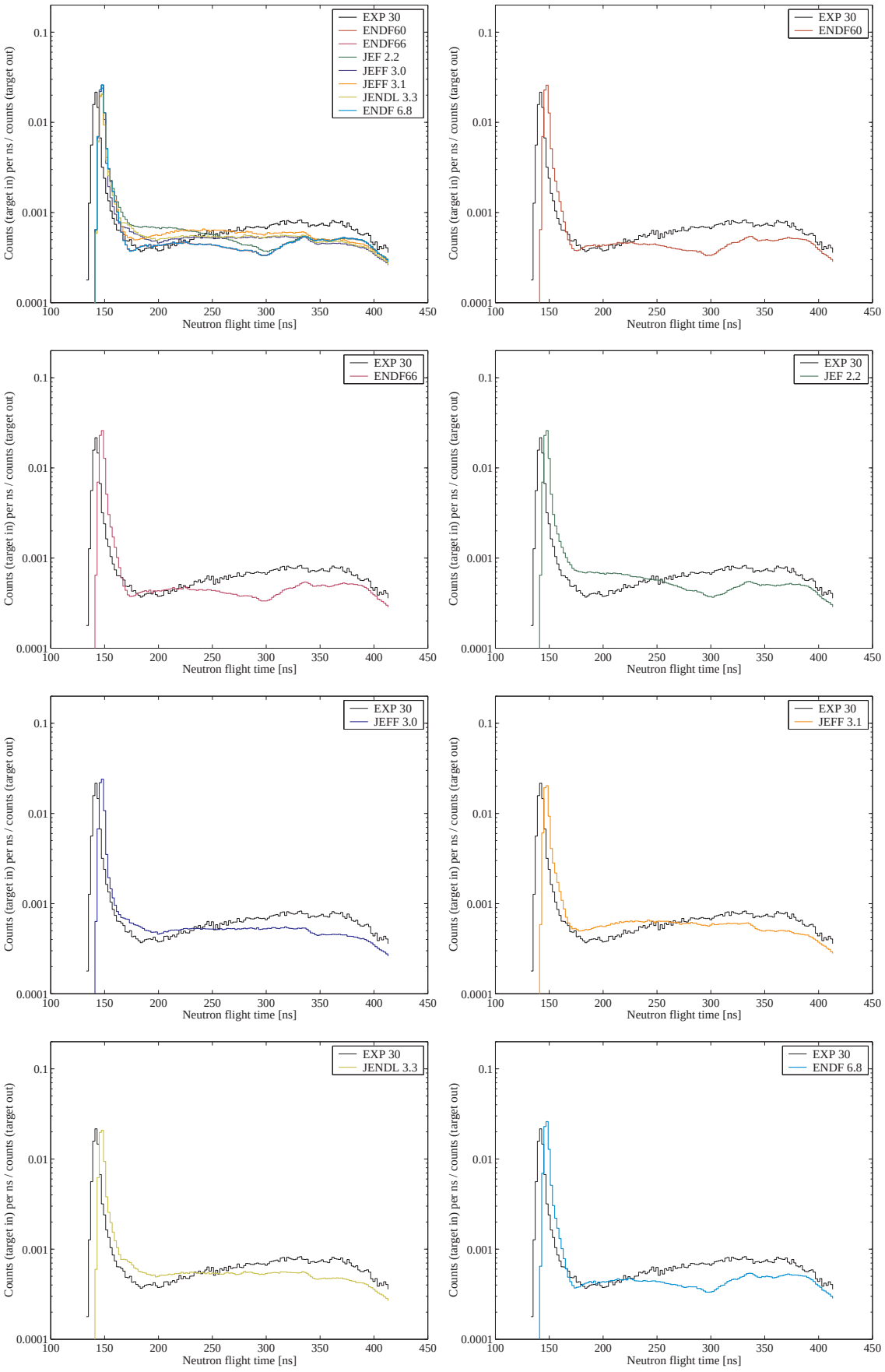

Figure 5.32: Experiment 30: Ti 3.5 mfp at 30 degrees with the Pilot B detector.

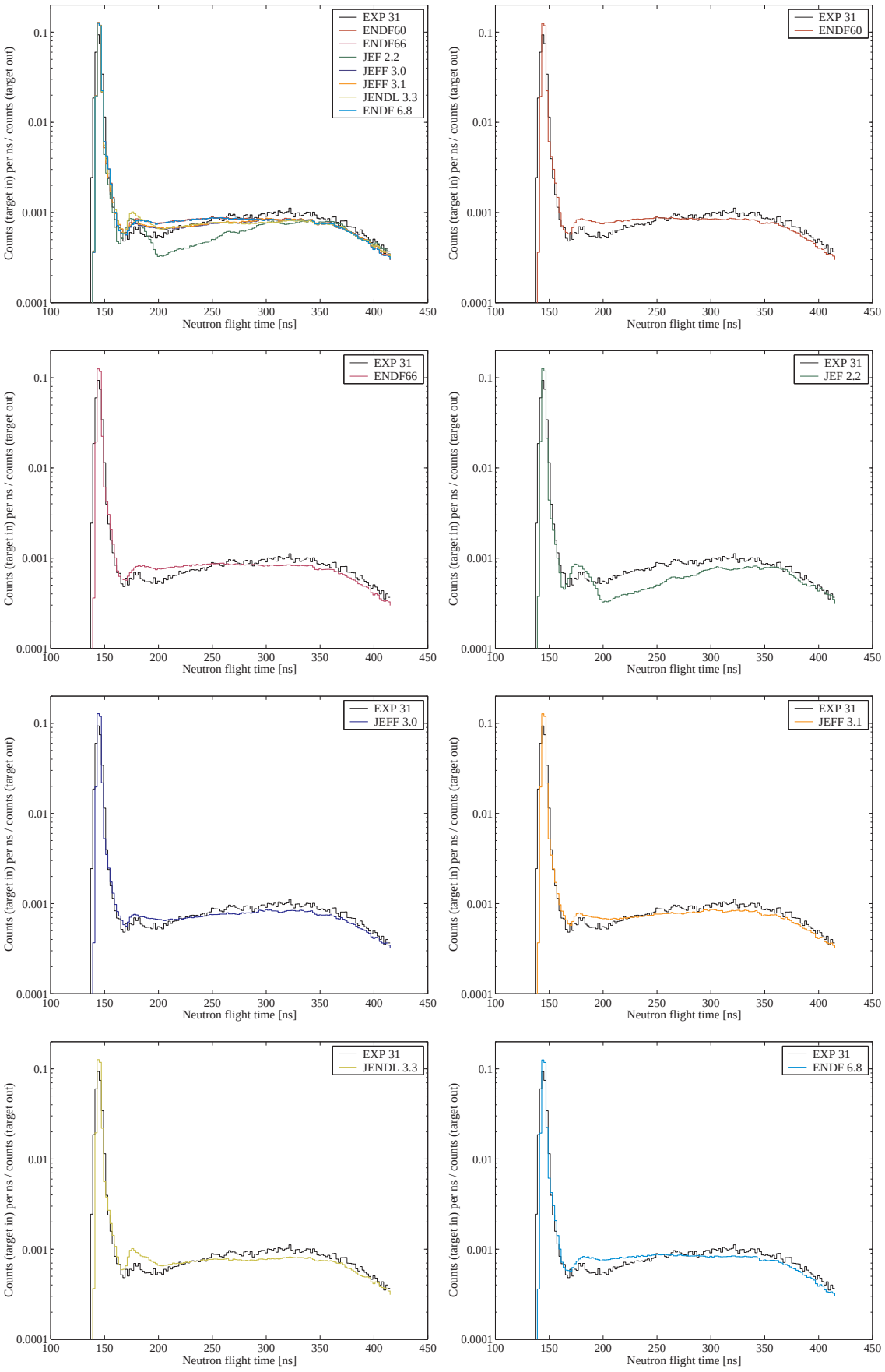

Figure 5.33: Experiment 31: Fe 0.9 mfp at 30 degrees with the NE213 detector.

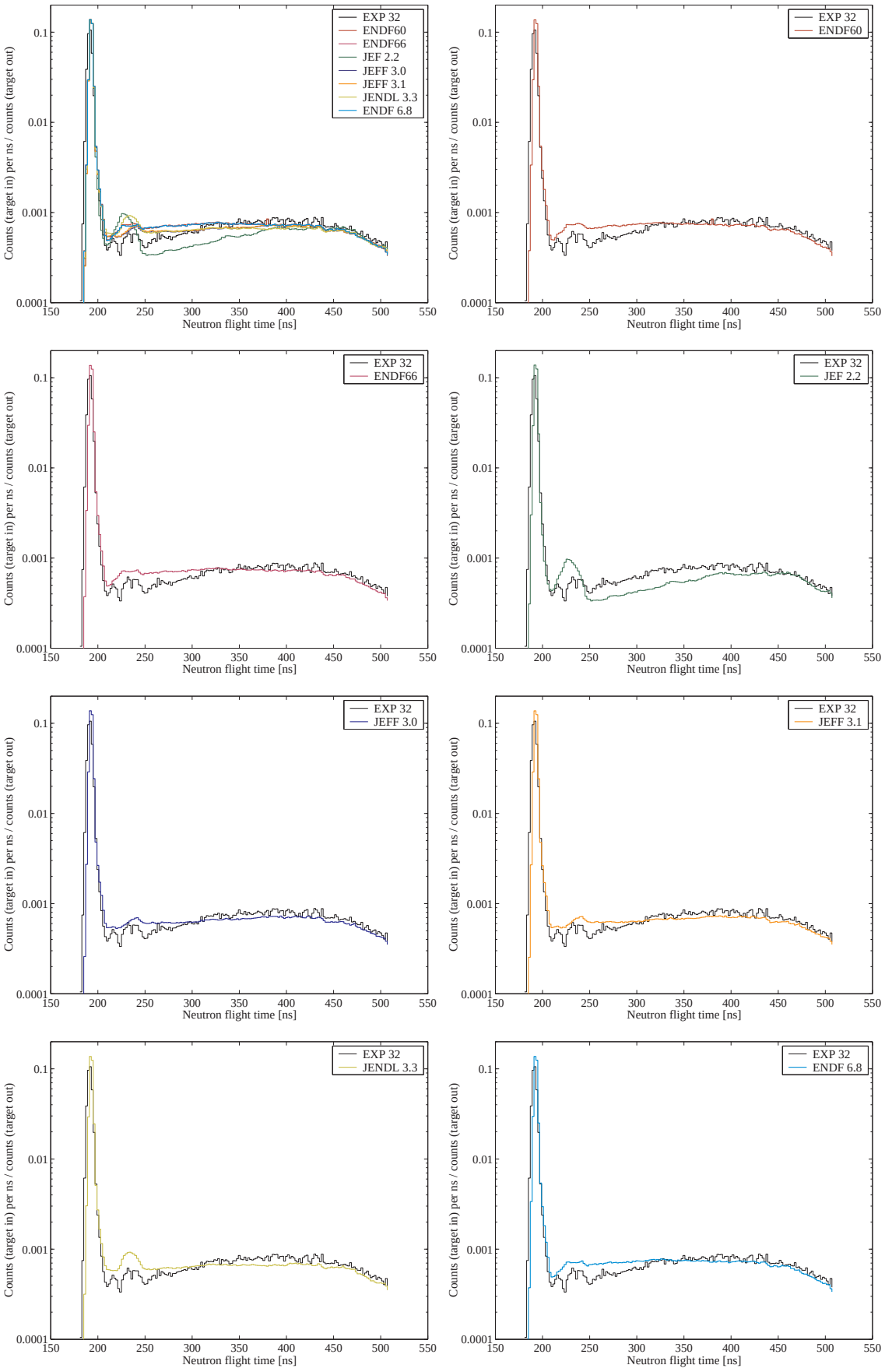

Figure 5.34: Experiment 32: Fe 0.9 mfp at 120 degrees with the NE213 detector.

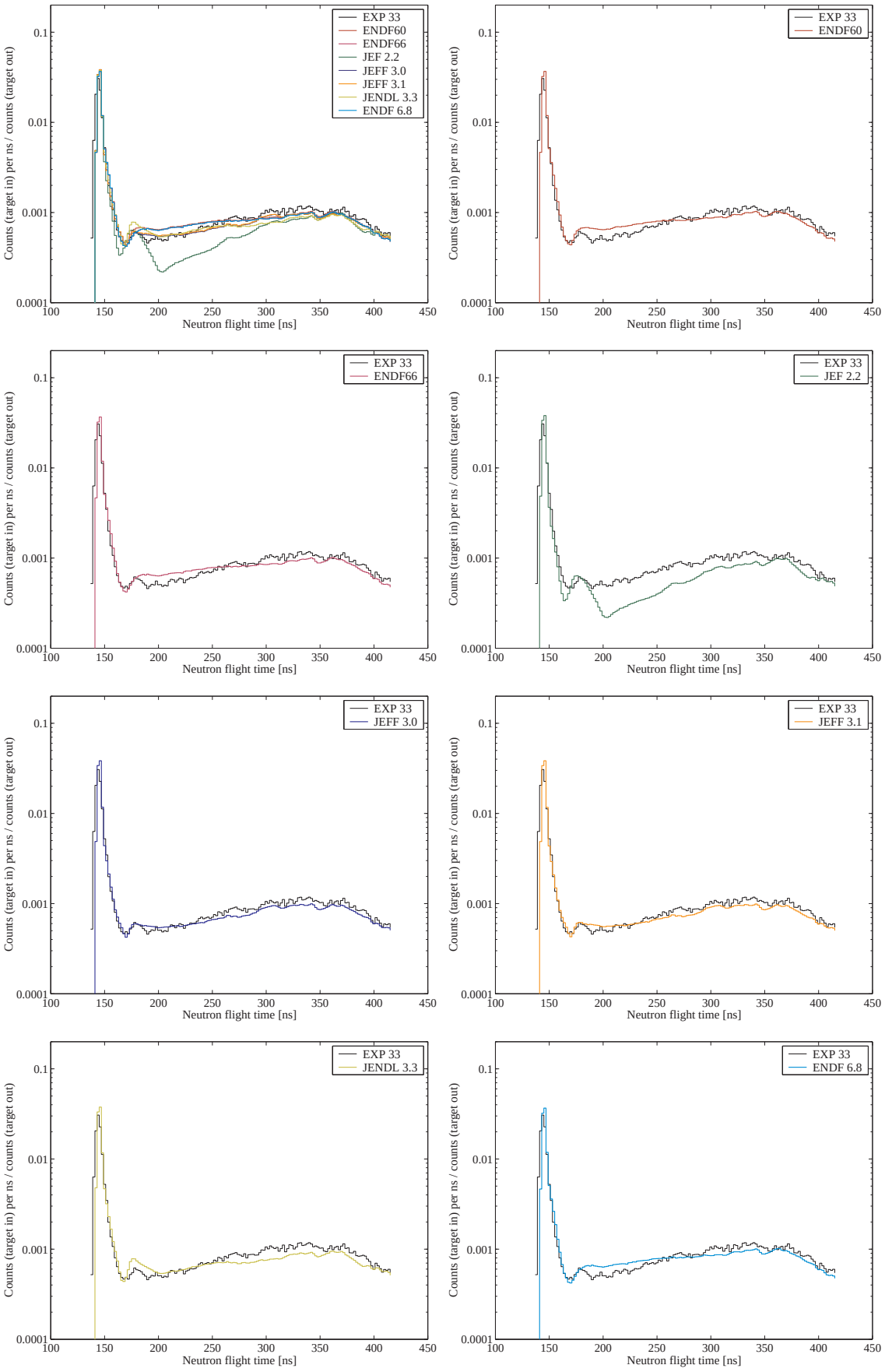

Figure 5.35: Experiment 33: Fe 2.9 mfp at 30 degrees with the NE213 detector.

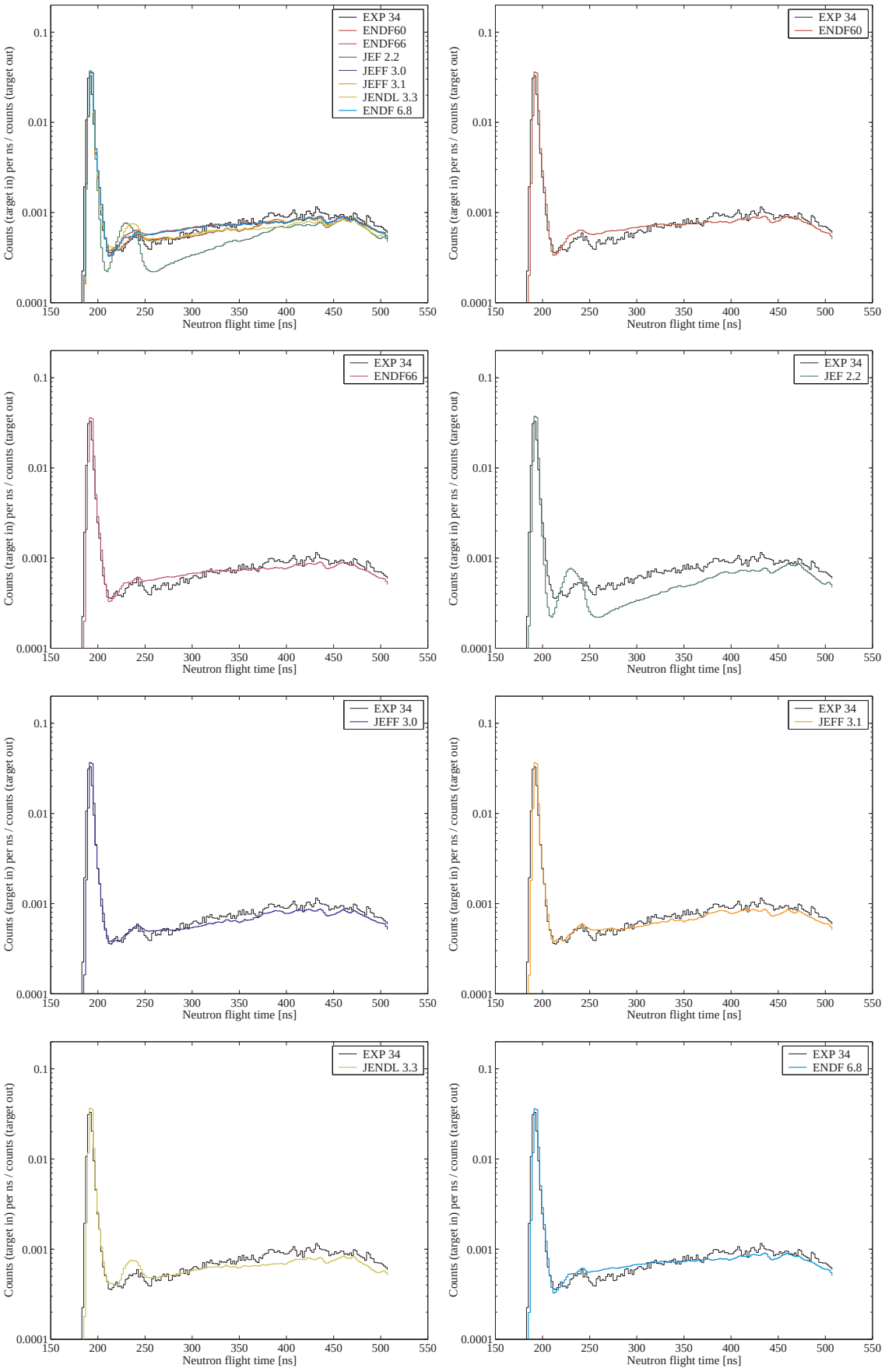

Figure 5.36: Experiment 34: Fe 2.9 mfp at 120 degrees with the NE213 detector.

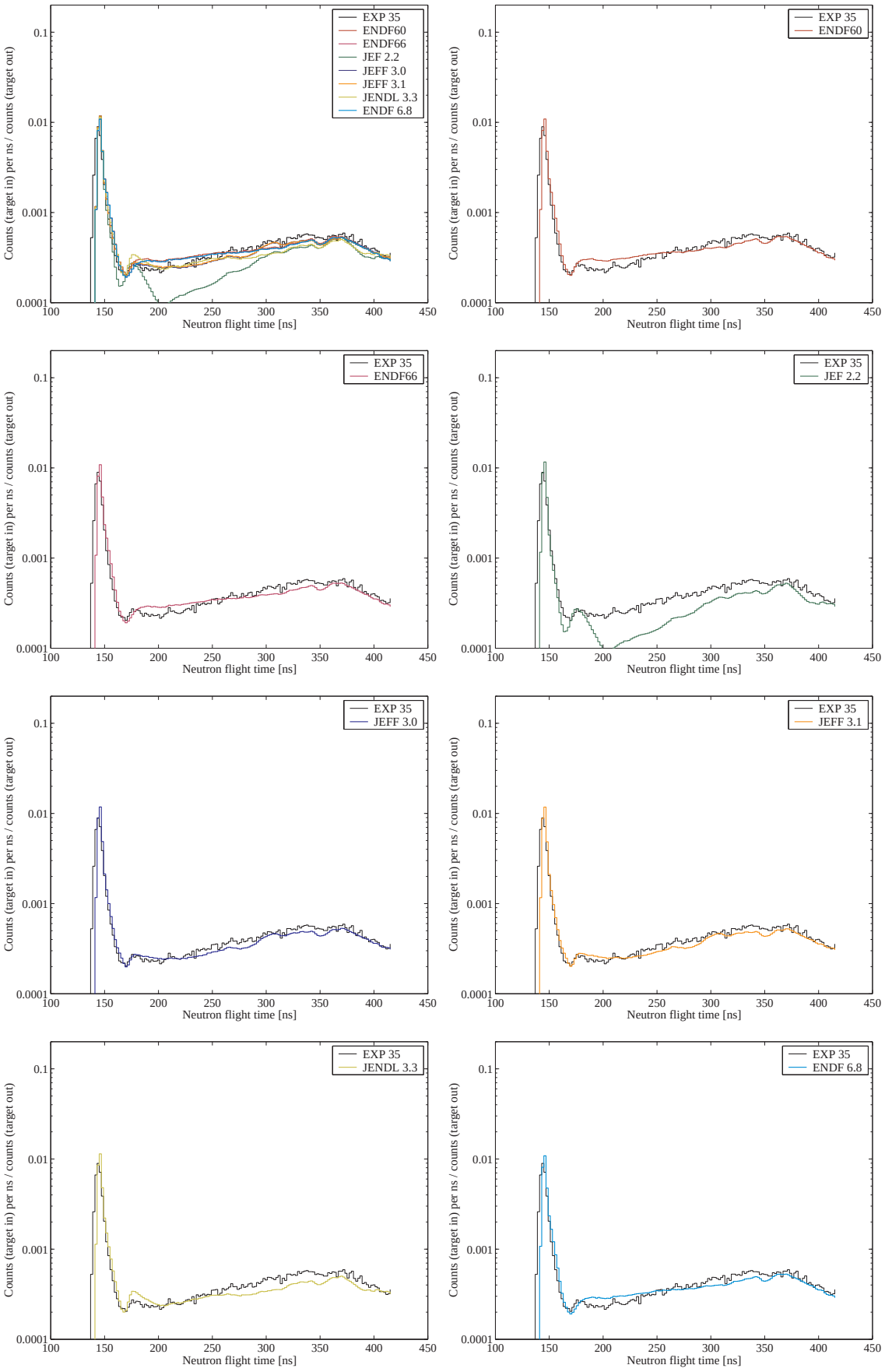

Figure 5.37: Experiment 35: Fe 4.8 mfp at 30 degrees with the NE213 detector.

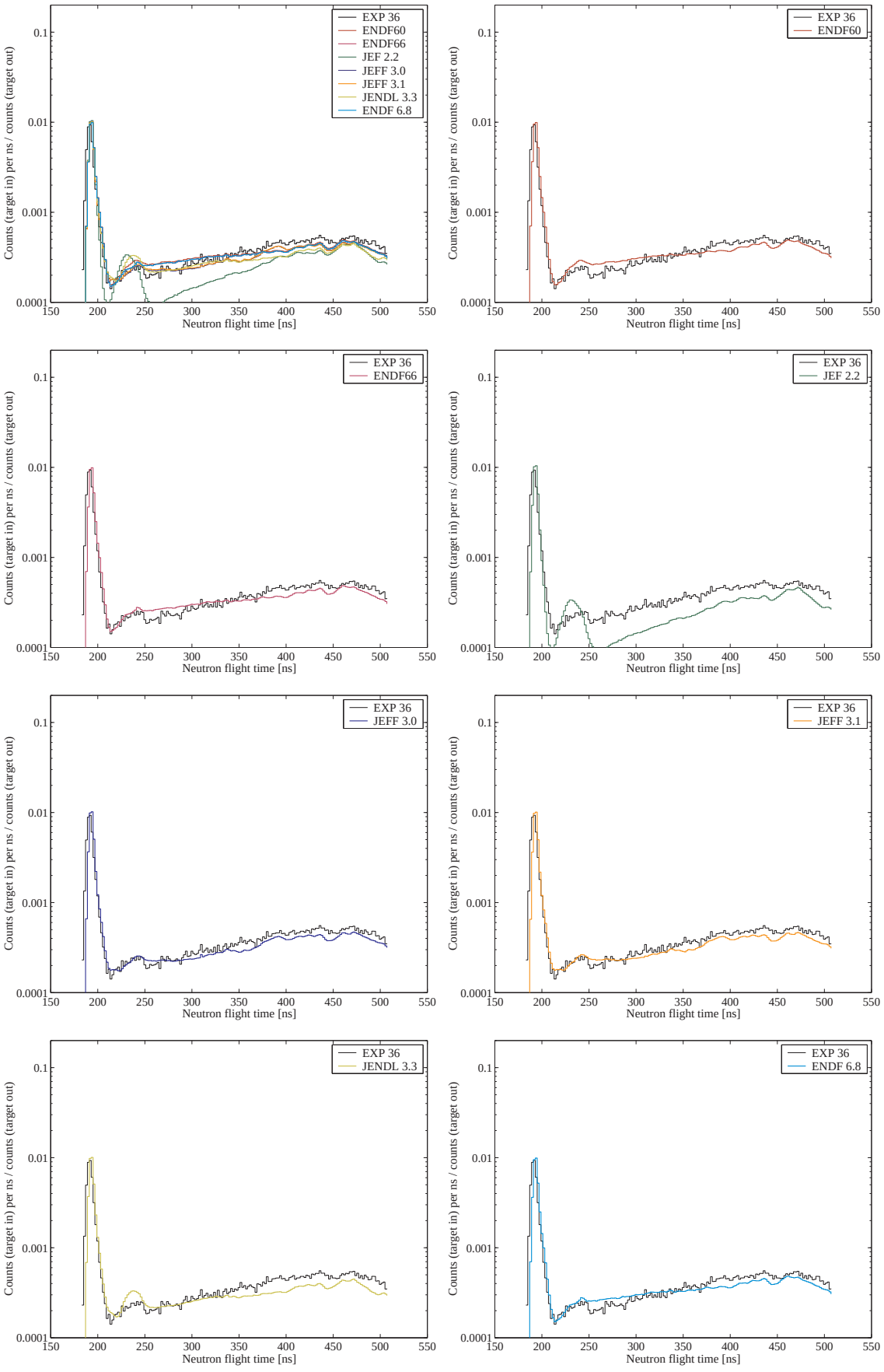

Figure 5.38: Experiment 36: Fe 4.8 mfp at 120 degrees with the NE213 detector.

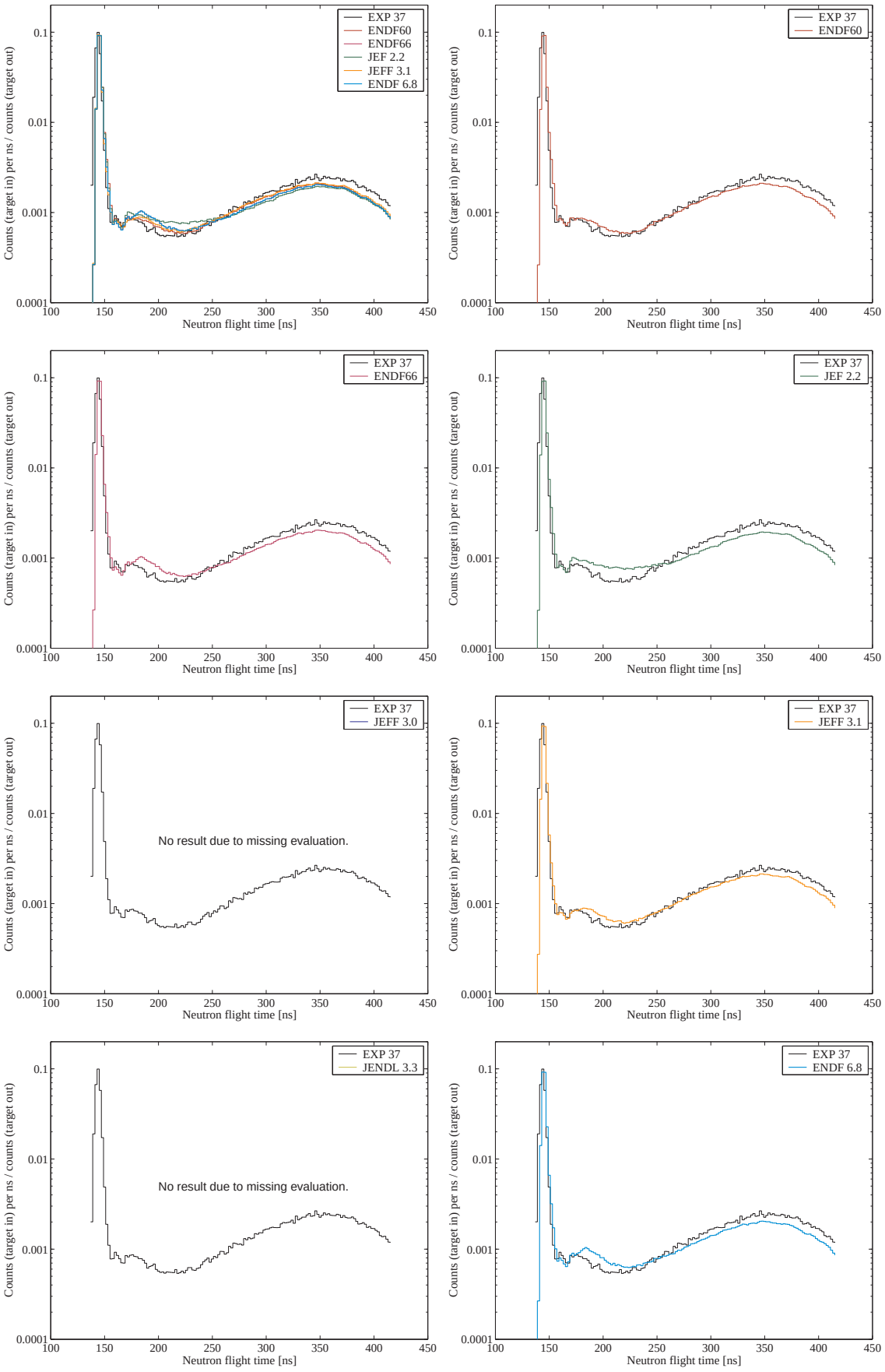

Figure 5.39: Experiment 37: Pb 1.4 mfp at 30 degrees with the NE213 detector.

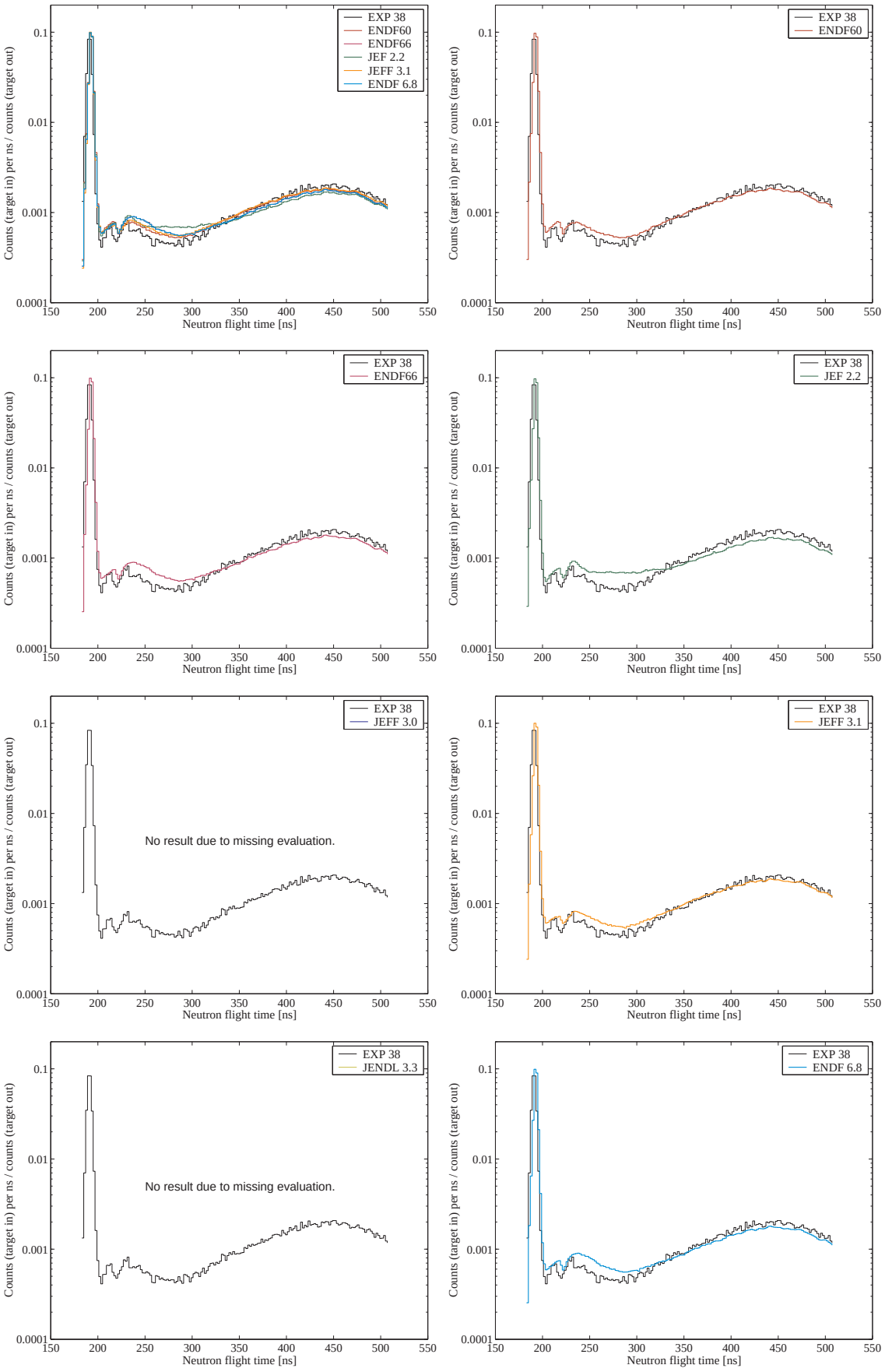

Figure 5.40: Experiment 38: Pb 1.4 mfp at 120 degrees with the NE213 detector.

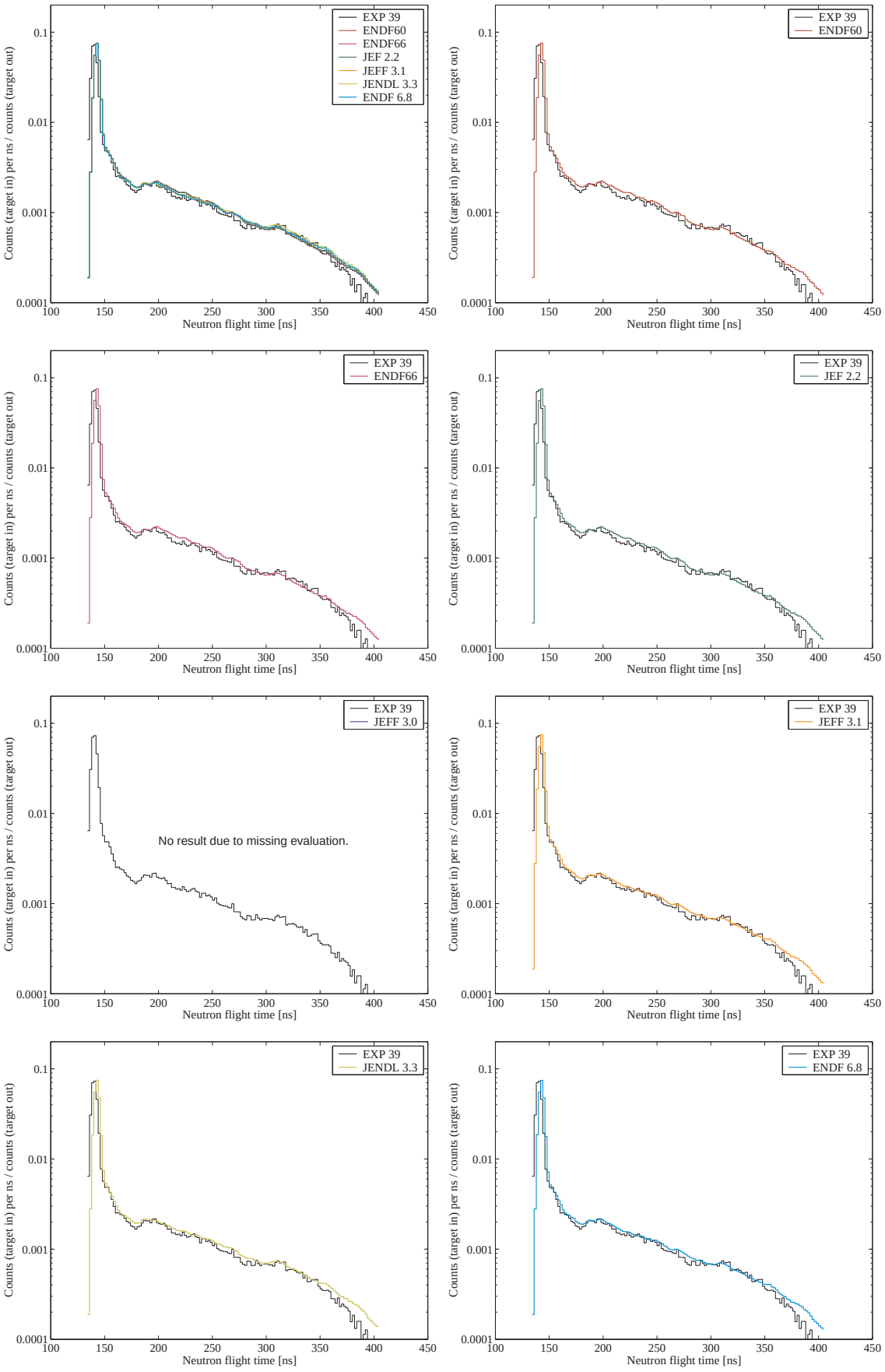

Figure 5.41: Experiment 39: H_2O 1.1 mfp at 30 degrees with the Pilot B detector.

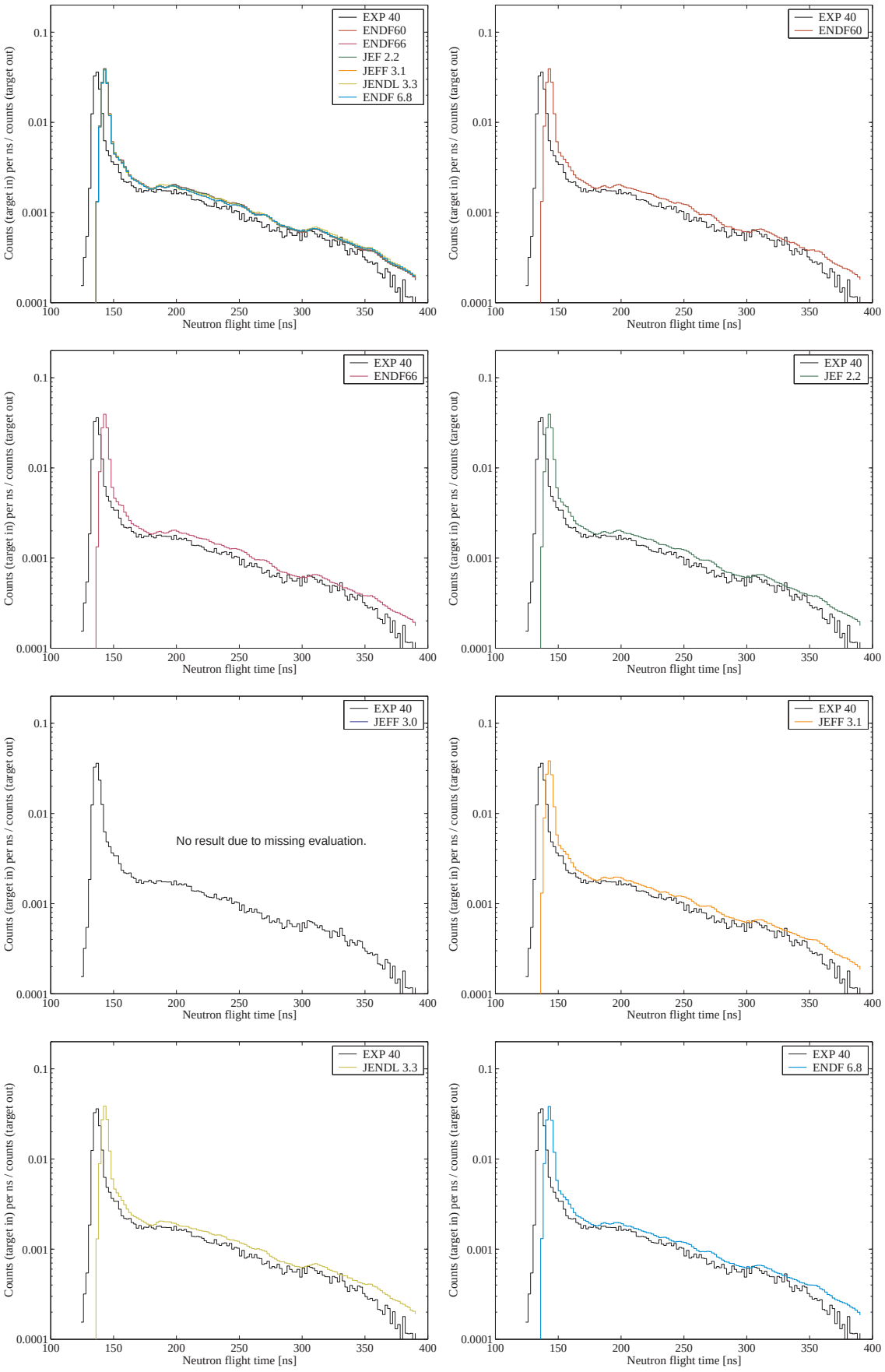

Figure 5.42: Experiment 40: H_2O 1.9 mfp at 30 degrees with the Pilot B detector.

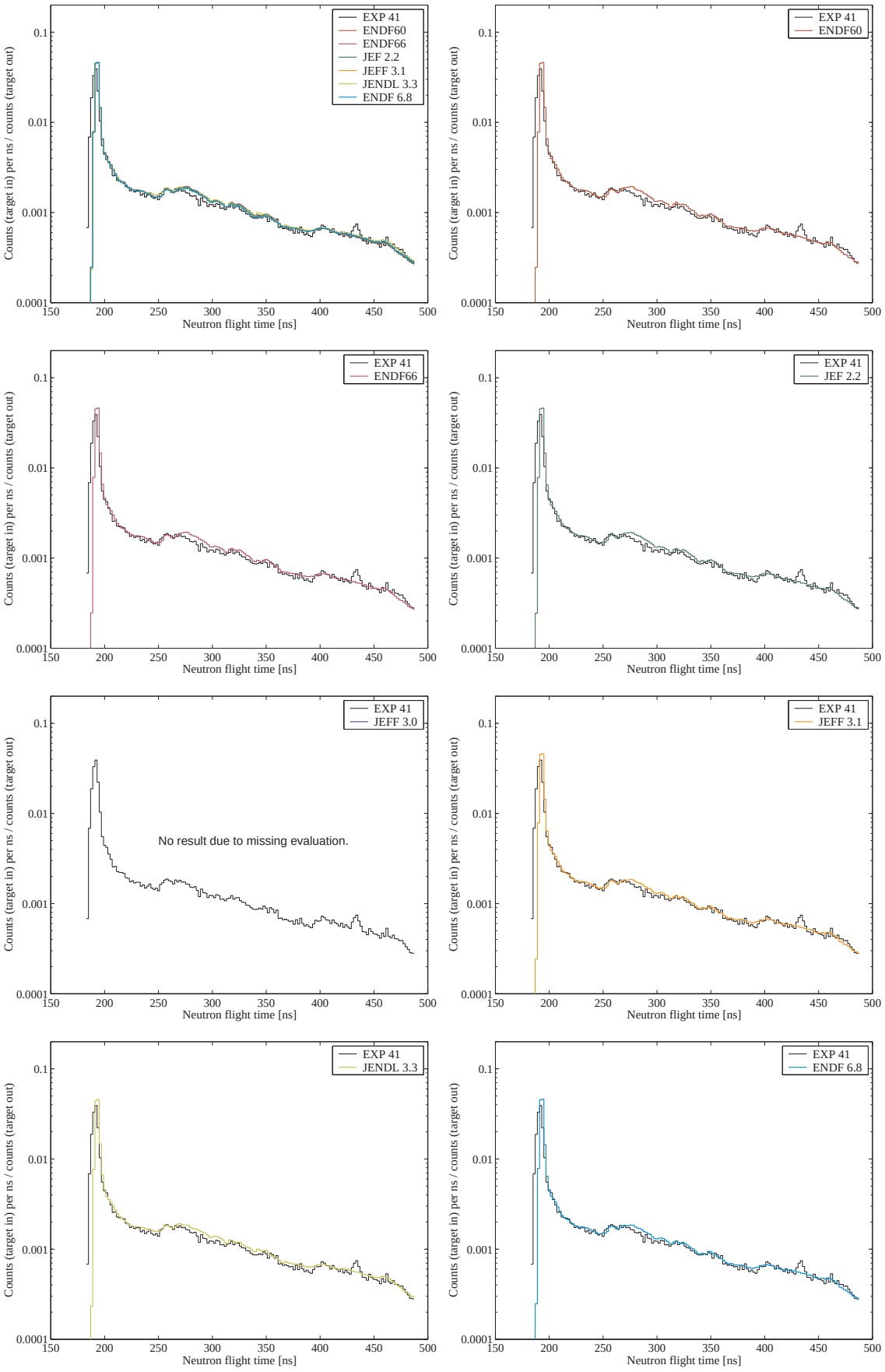

Figure 5.43: Experiment 41: H_2O 1.9 mfp at 120 degrees with the NE213 detector.

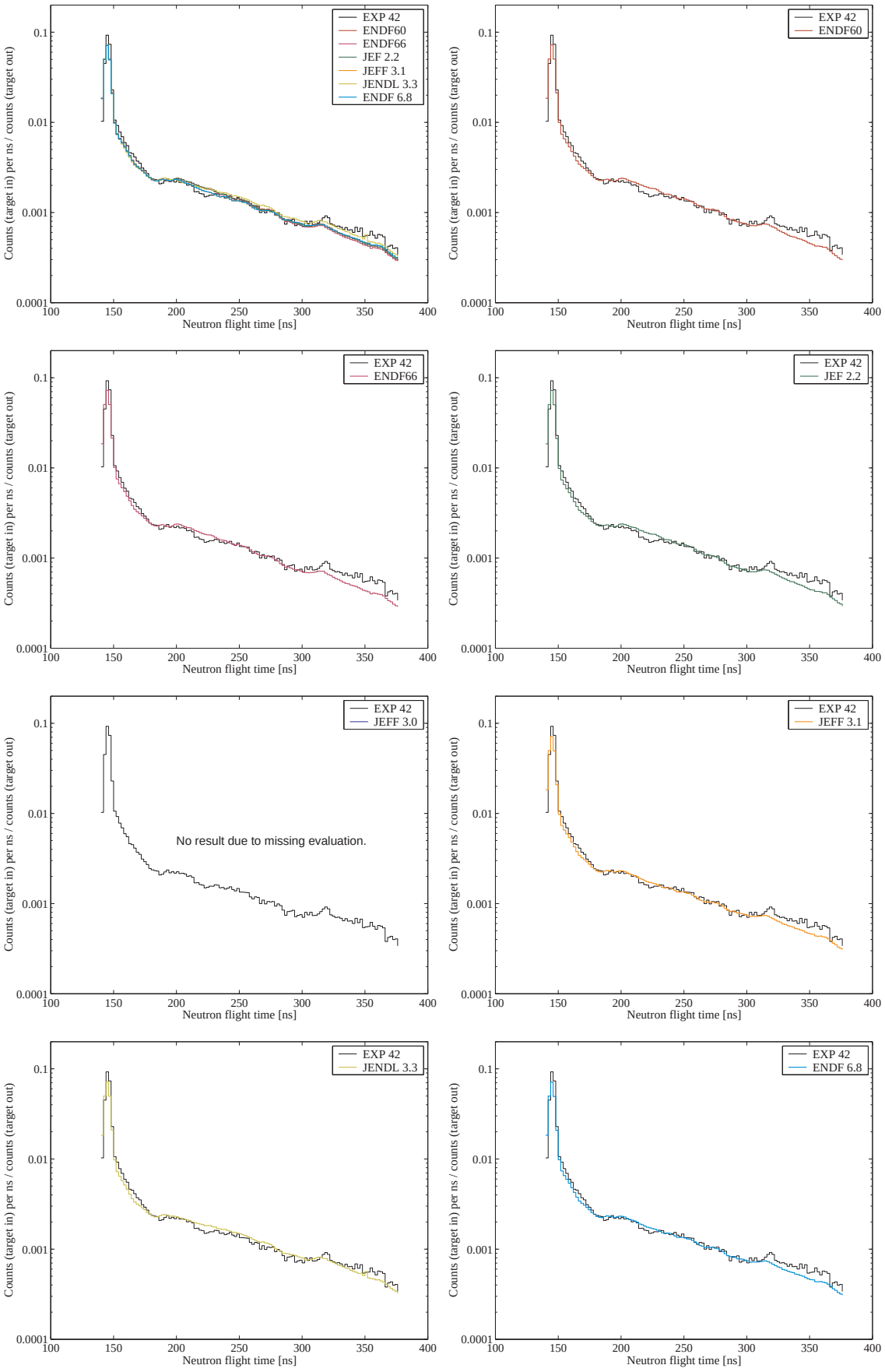

Figure 5.44: Experiment 42: D_2O 1.2 mfp at 30 degrees with the Pilot B detector.

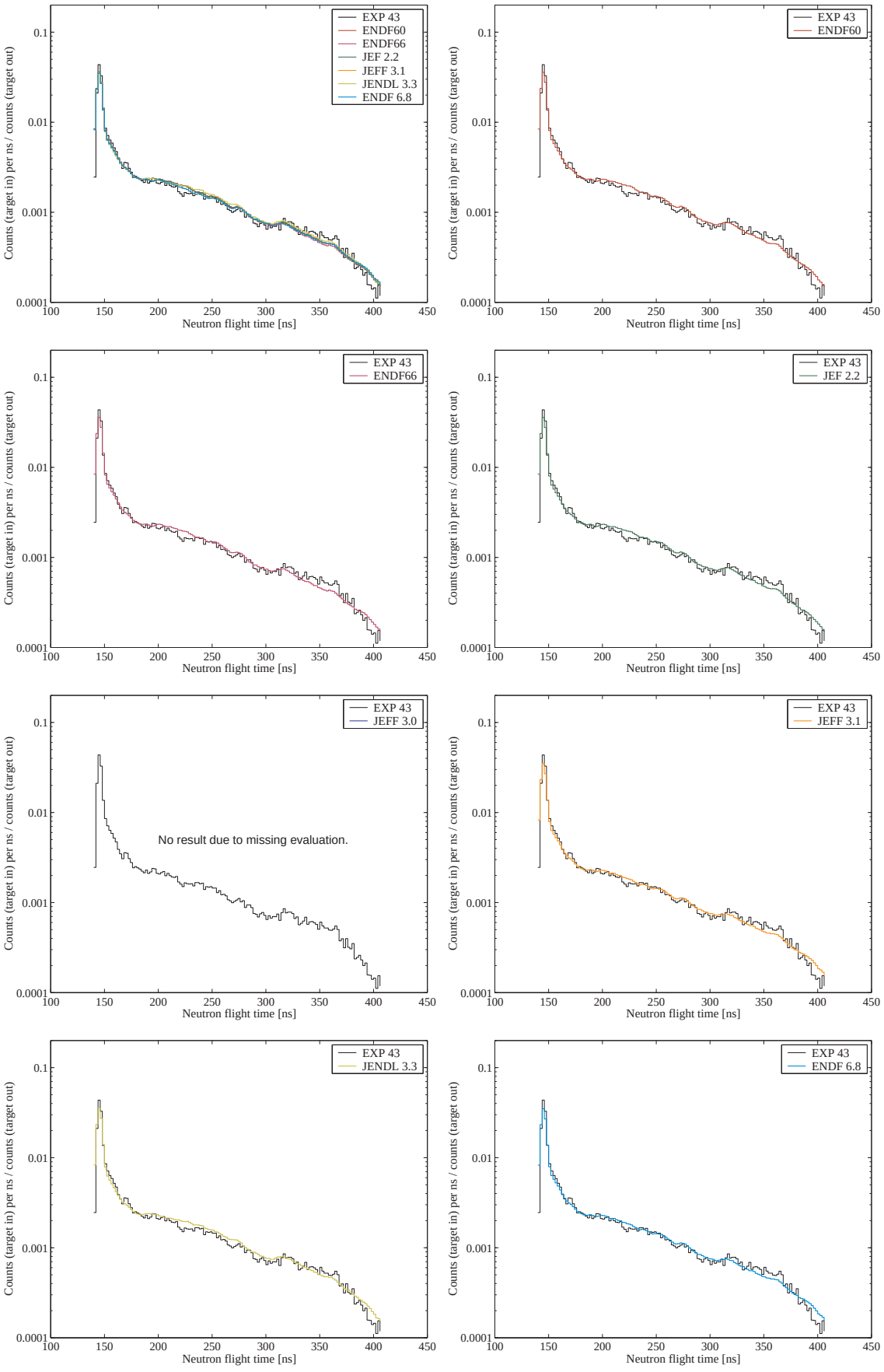

Figure 5.45: Experiment 43: D_2O 2.1 mfp at 30 degrees with the Pilot B detector.

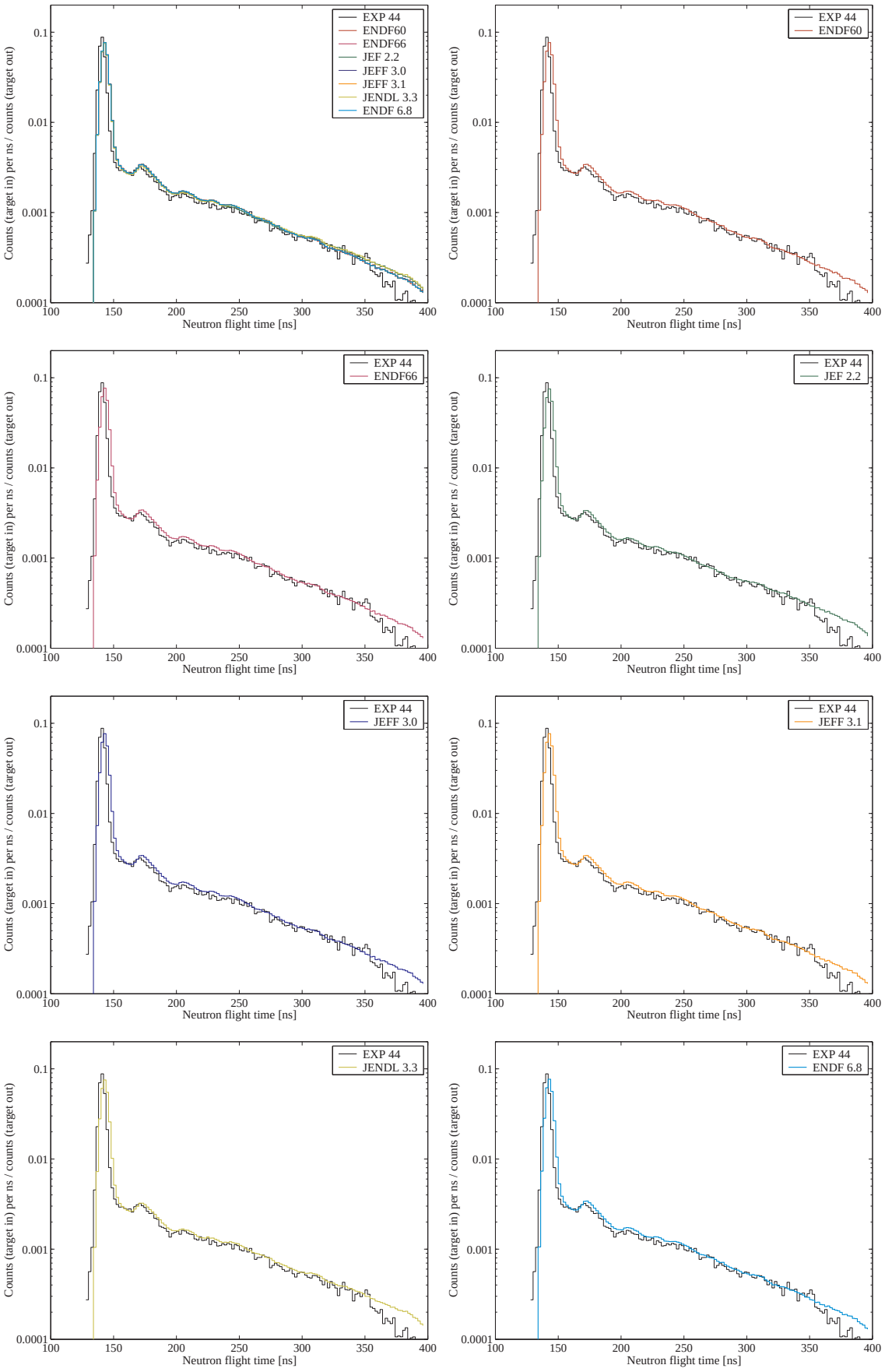

Figure 5.46: Experiment 44: Polyethylene 0.7 mfp at 30 degrees with the Pilot B detector.

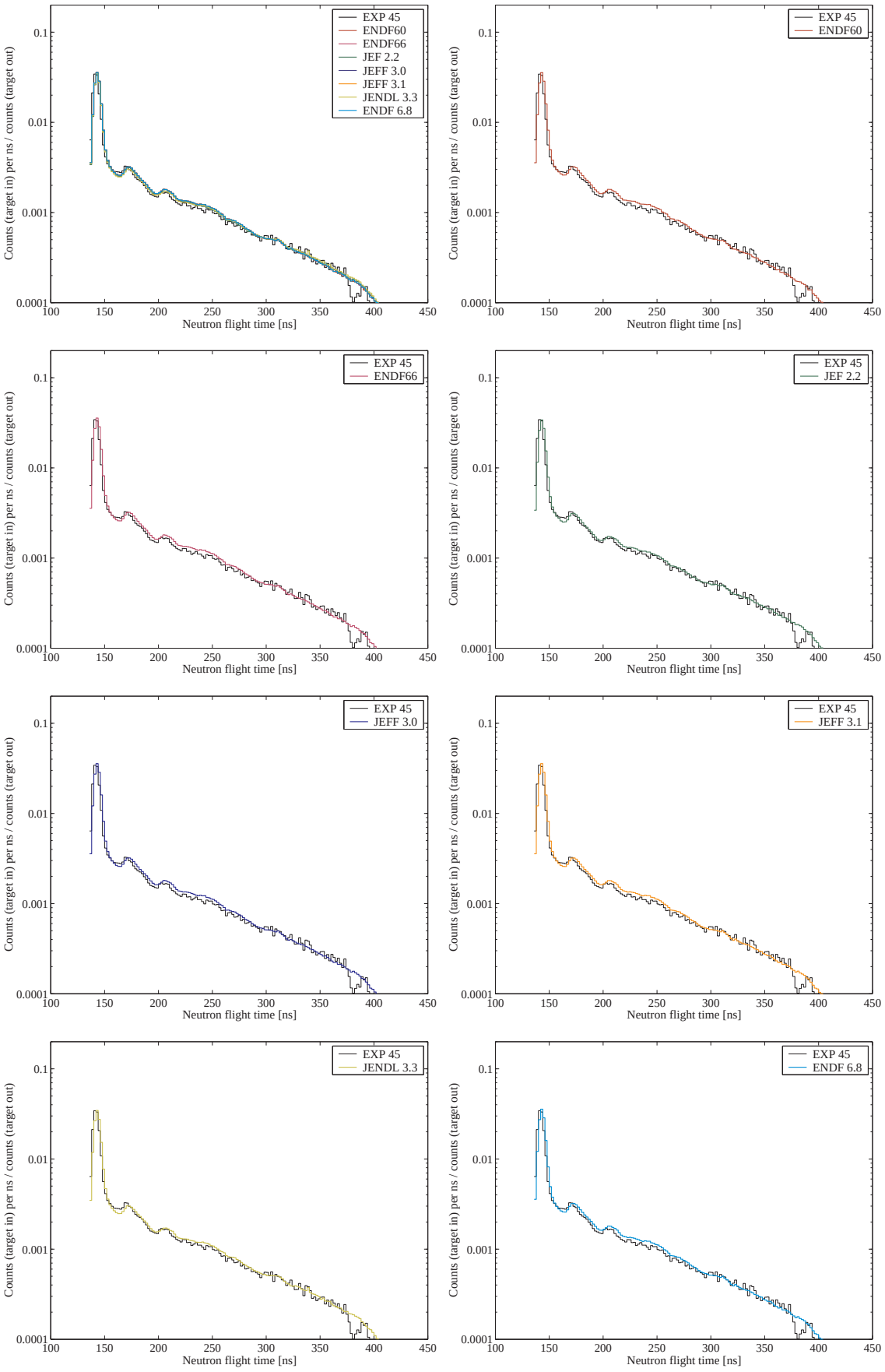

Figure 5.47: Experiment 45: Polyethylene 1.6 mfp at 30 degrees with the Pilot B detector.

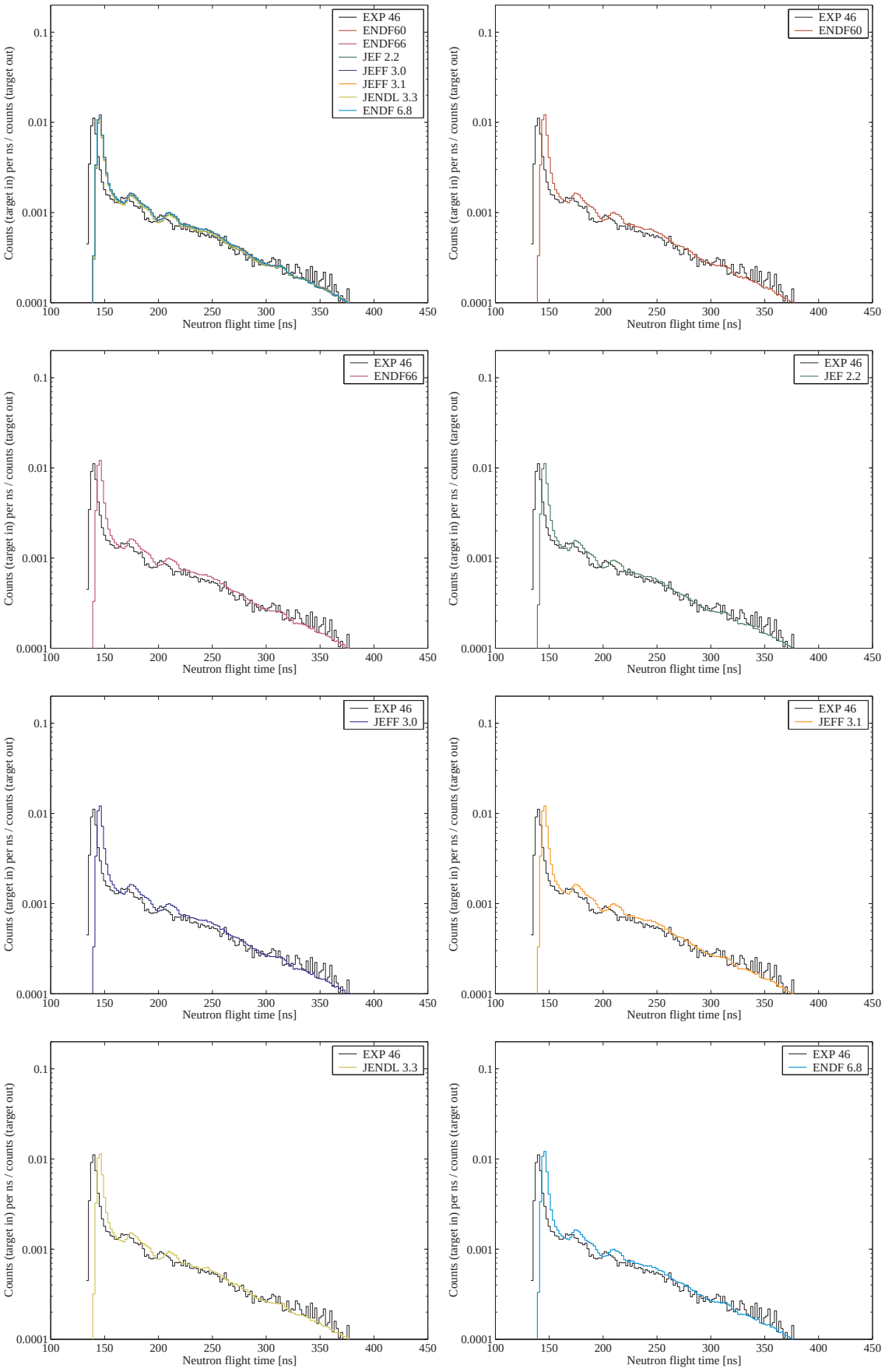

Figure 5.48: Experiment 46: Polyethylene 3.0 mfp at 30 degrees with the Pilot B detector.

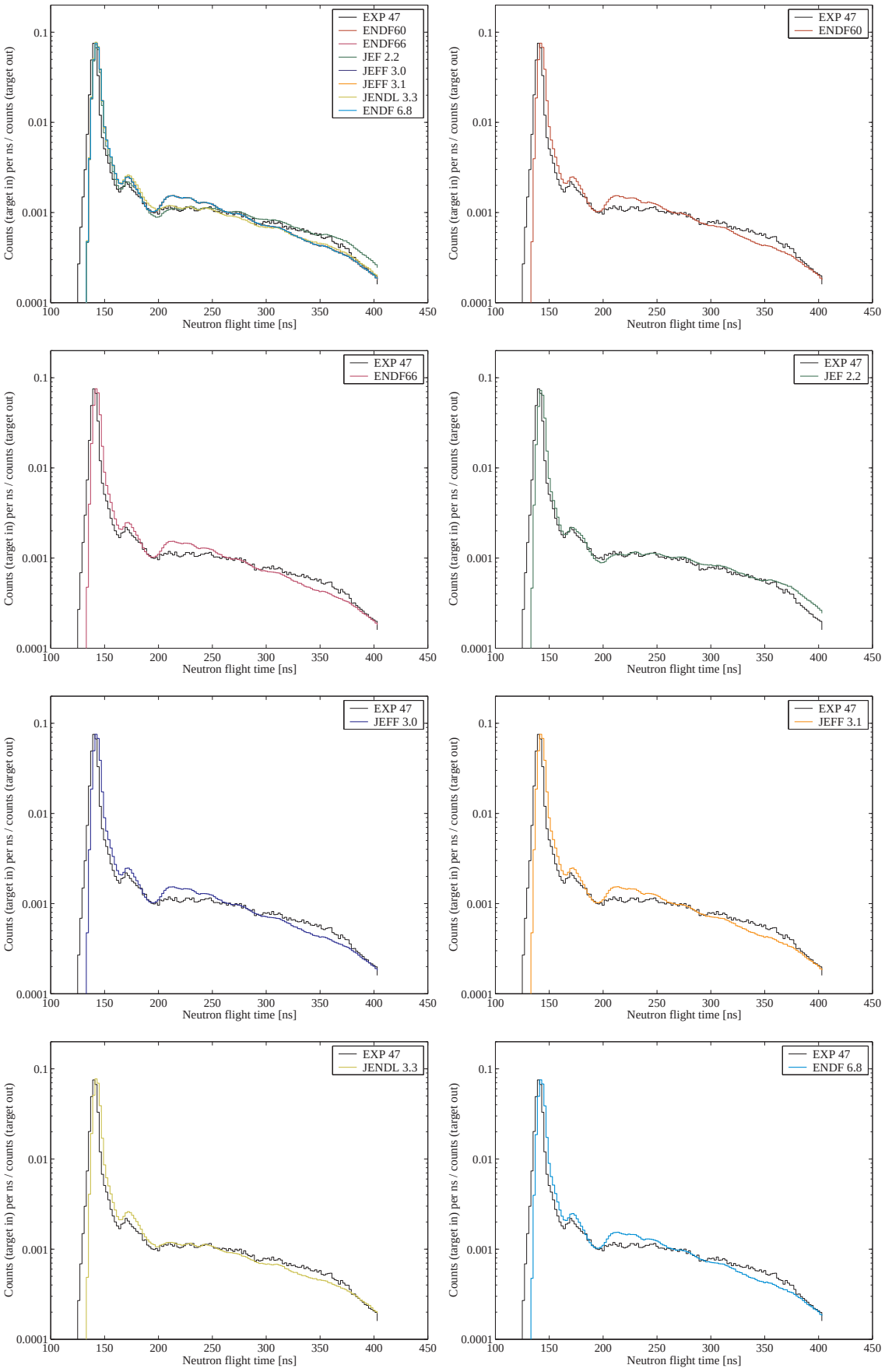

Figure 5.49: Experiment 47: Teflon 0.9 mfp at 30 degrees with the Pilot B detector.

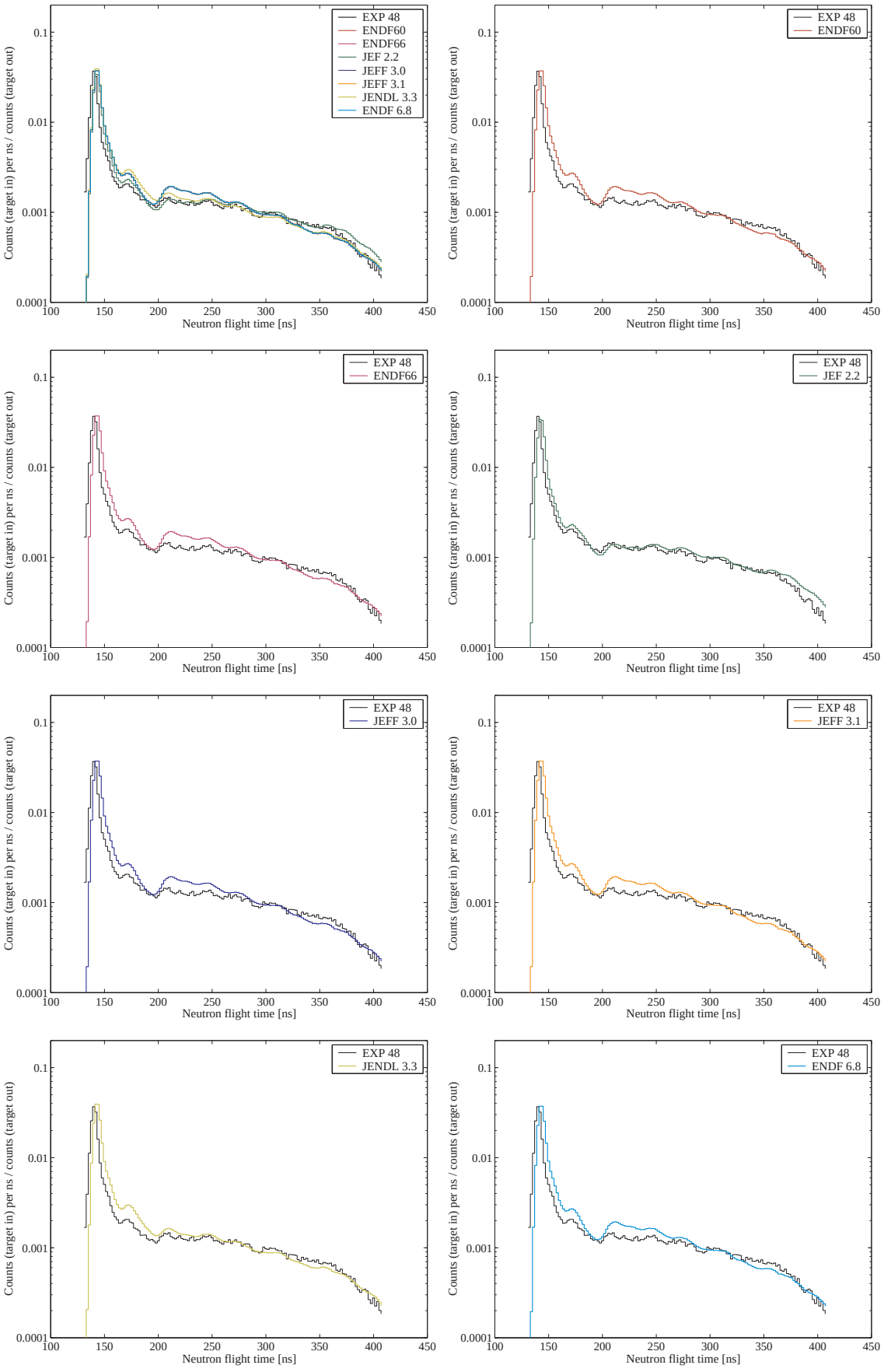

Figure 5.50: Experiment 48: Teflon 1.8 mfp at 30 degrees with the Pilot B detector.

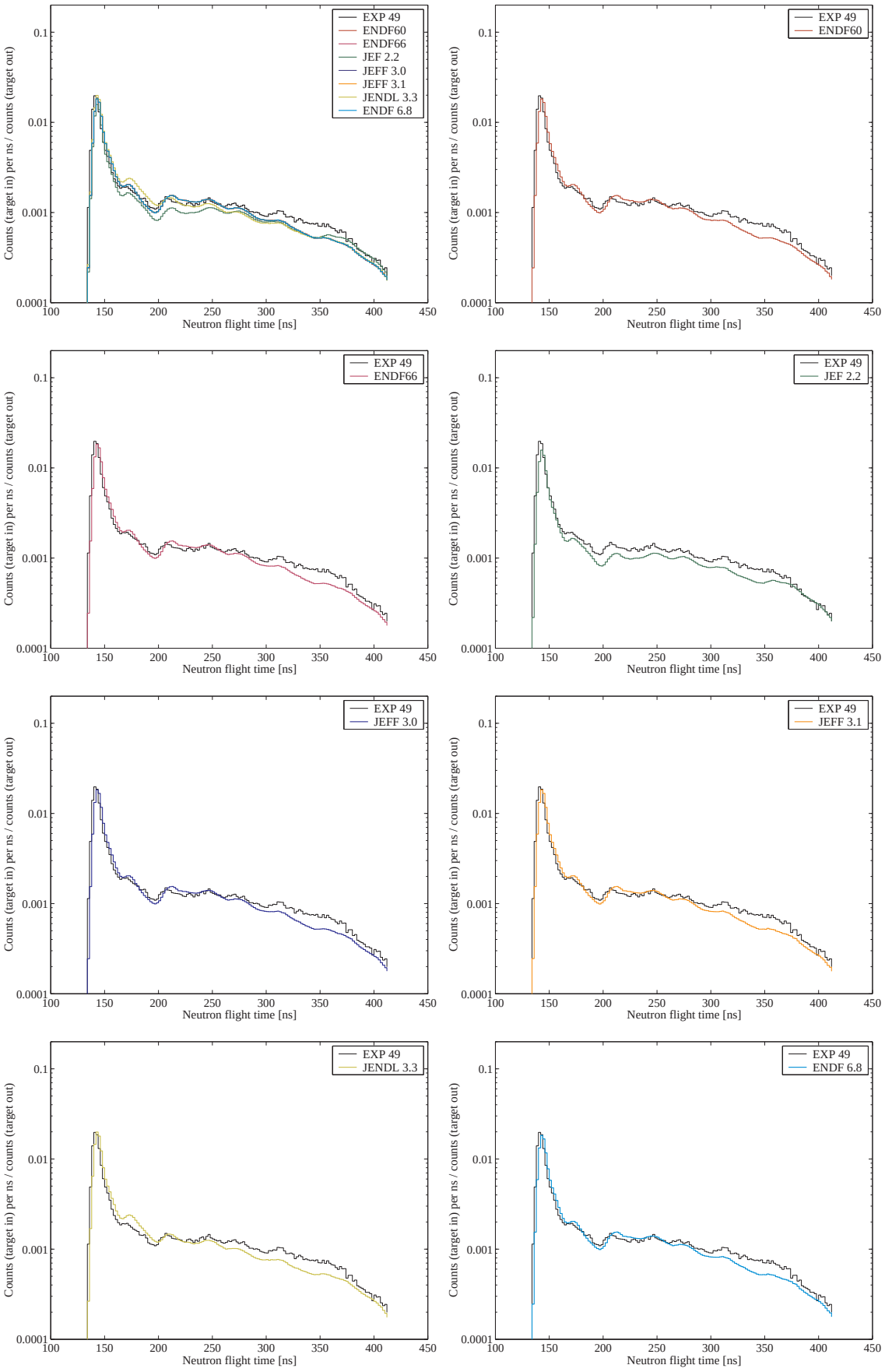

Figure 5.51: Experiment 49: Teflon 2.9 mfp at 30 degrees with the Pilot B detector.

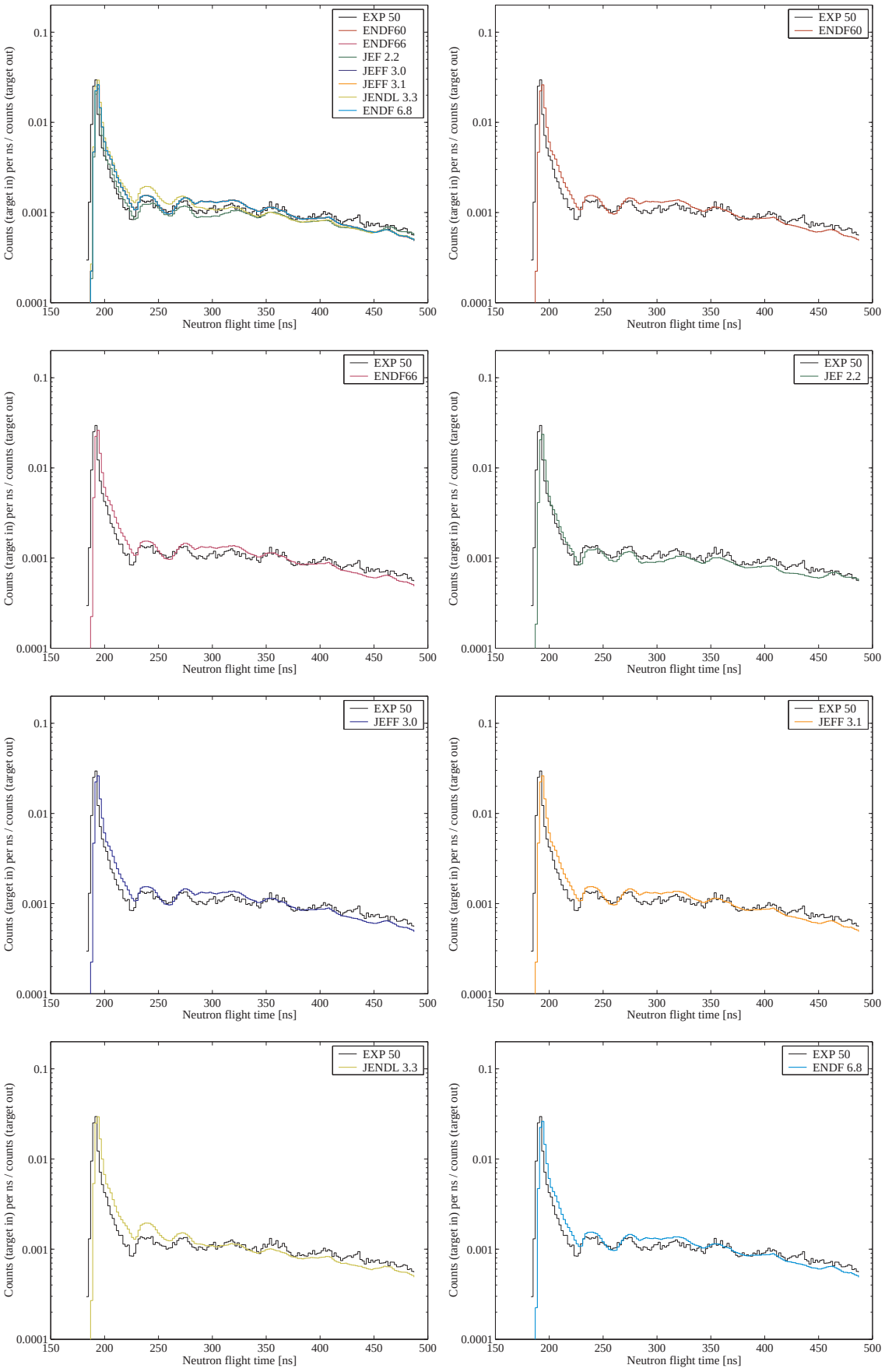

Figure 5.52: Experiment 50: Teflon 2.9 mfp at 120 degrees with the NE213 detector.

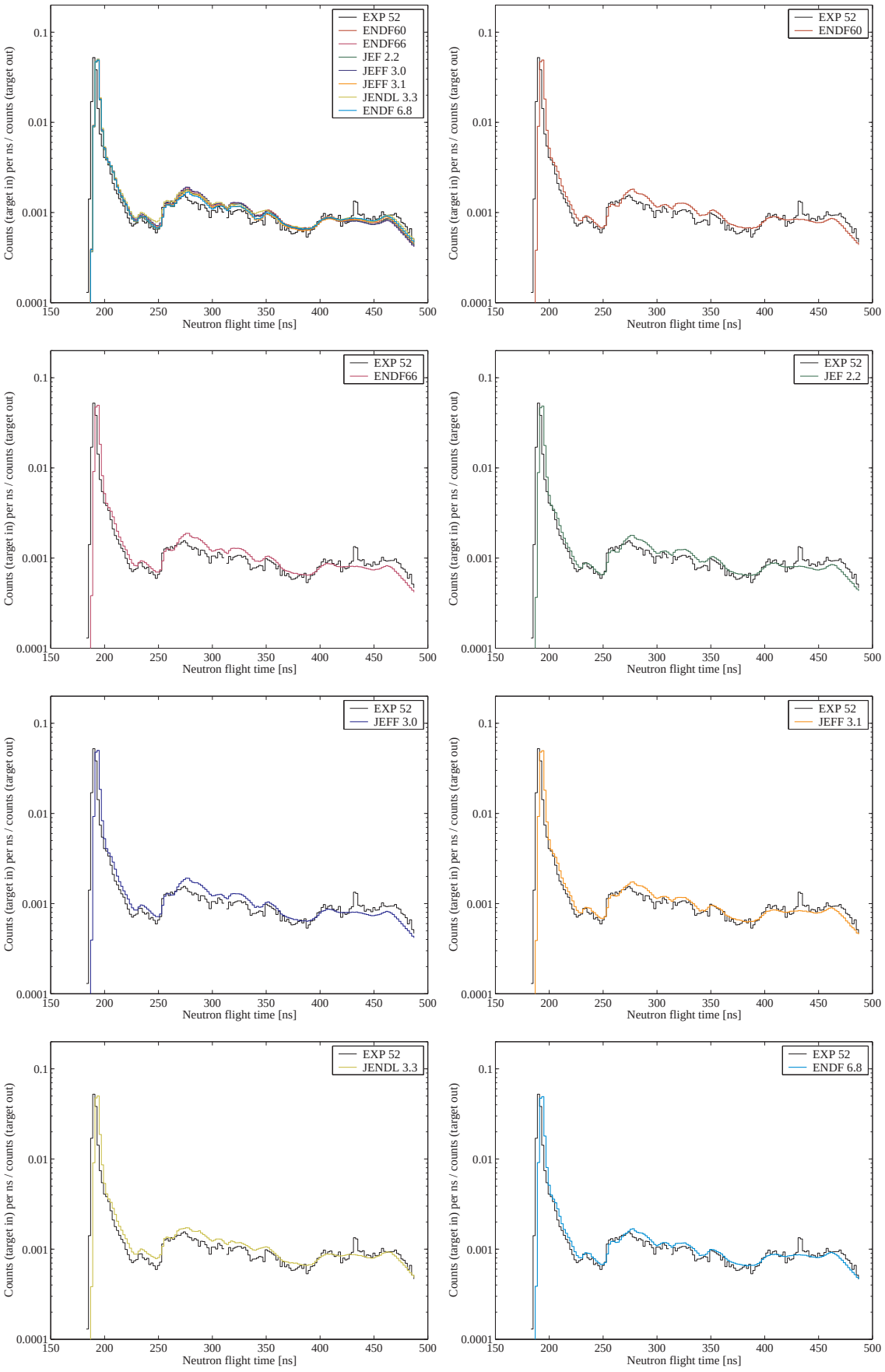

Figure 5.53: Experiment 52: Concrete 2.0 mfp at 120 degrees with the NE213 detector.

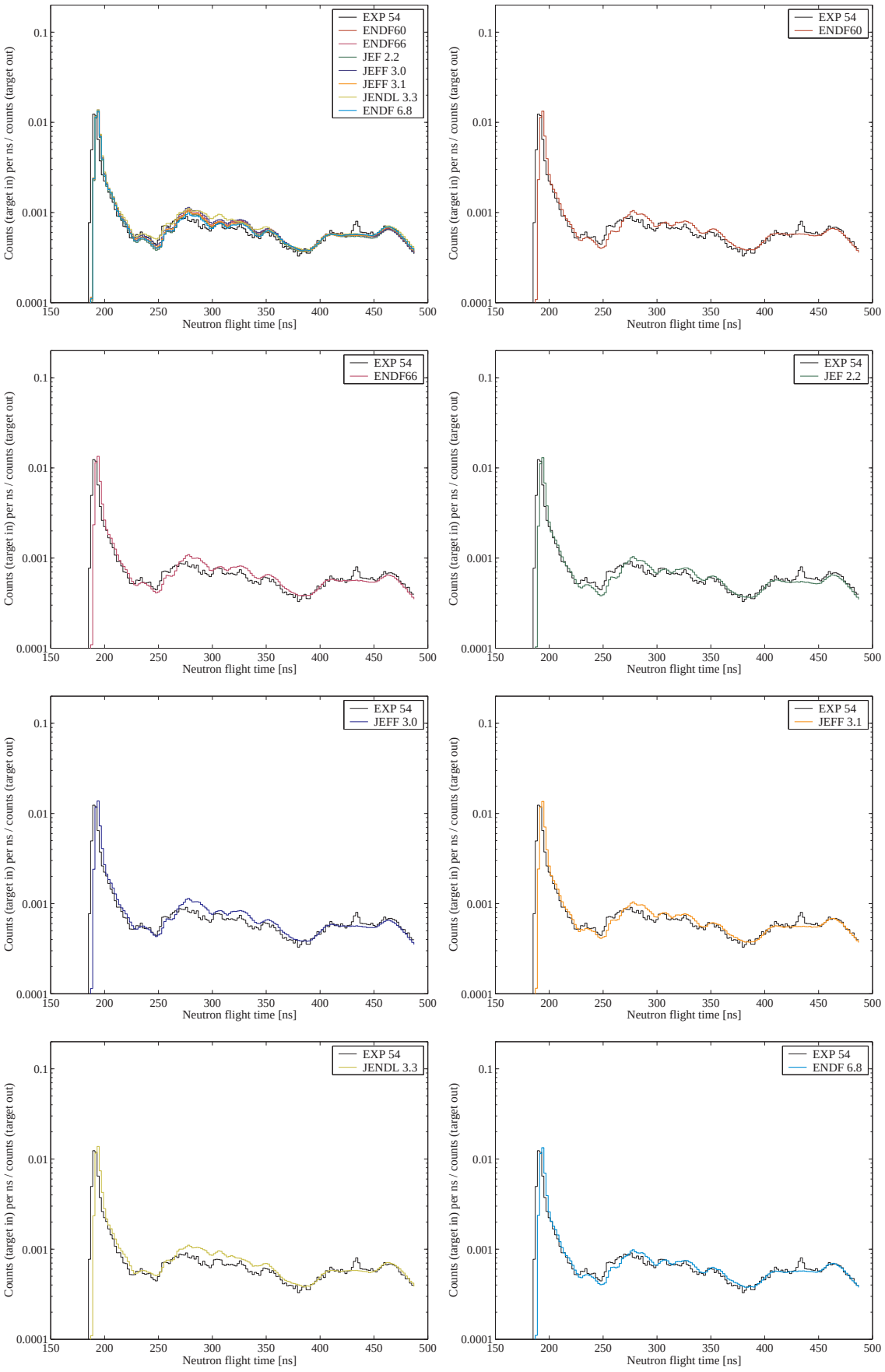

Figure 5.54: Experiment 54: Concrete 3.8 mfp at 120 degrees with the NE213 detector.

Appendix A

Updates to NJOY

```
*ident updlg1
*/ Increase the number of significant digits in unresr and purr
*/ for the purpose of testing the probability tables.
*d unresr.202
           if (iprint.eq.1) write(nsyso,'(1x,1p,8e14.6)')
*d purr.1797
     &  15x,''total'',7x,''elastic'',7x,''fission'',7x,
*d up42.12
      if (iprint.gt.0) write(nsyso,'(i6,1p,4e14.6)')
*d purr.2256,2258
     &  ''  bkgd'',1p,4e14.6/''  infd'',1p,4e14.6/
     &  ''  aver'',1p,4e14.6/''  pcsd'',0p,4f14.2/
     &  ''  nres'',i14)')
*d purr.2265,2266
     &  9x,''temp'',6x,''sig0'',6x,''p0 total'',7x,
     &  ''elastic'',7x,''fission'',7x,''capture'',6x,
*d purr.2280
              write(nsyso,'(3x,1p,2e10.3,5e14.6)')
*d up84.121
     &           '('' tmax'',1p,e11.3,1p,10e14.6/(16x,10e14.6))')
*d up84.124
     &           '('' prob'',1p,e11.3,1p,10e14.6/(16x,10e14.6))')
*d up84.127
           write(nsyso,'(1x,a,1x,1p,e11.3,10e14.6/(16x,10e14.6))')
*d purr.2338,2339
     &  9x,''temp'',6x,''sig0'',6x,''p0 total'',7x,''elastic'',
     &  7x,''fission'',7x,''capture'',6x,''p1 total'')')
*d purr.2372
              write(nsyso,'(3x,1p,2e10.3,5e14.6)')
*ident updlg2
*/ Pu239 of JEF 2.2 has a problem in purr ('not enough scratch space')
*/ up104 fixes this (by increasing it to 12000), but to be sure we
*/ increase if to 50000
*d up104.5
      maxscr=50000
*ident updlg3
*/ updates up92 and up99 are the same so one of them may be removed
*d up92.6
*d up92.8
```

Appendix B

Contents of ALEPH-LIB

Table B.1 gives an overview of the content of the JEFF 3.1 MCNP(X) library within ALEPH-LIB. The entries in each of the columns of this table are described as follows:

Nuclide: this is the nuclide ZAMID identification number (similar to the ZAID identification used by MCNP(X)). The ZAMID number is the ORIGEN identification number of the isotope (using the element number Z, the atomic mass number A and the metastable state M which is either 0 or 1):

$$\mathtt{ZAMID} = 10000\,\mathtt{Z} + 10\,\mathtt{A} + \mathtt{M} = 10\,\mathtt{ZAID} + \mathtt{M} \tag{B.0.1}$$

E_{max}: the maximum incident neutron energy for that data file.

GPD: this column indicates whether or not photon-production data are included.

CP: this column indicates whether or not charged particle production data are included, and if so for which type of particles.

$\bar{\nu}$: this column indicates the type of fission nu data that is included for a fissionable material. "tot" means that only total nu data are given and "both" means that prompt and total nu are given.

DN: this column indicates whether or not delayed neutron data are included.

T [K]: this column gives the temperatures for which library files exist.

Probability tables: this column indicates if the library files have unresolved resonance probability tables and gives the reason why such probability tables are not included.

Table B.1: JEFF 3.1 library files overview.

Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
10010	150	yes	d	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
10020	150	yes	p,t	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
10030	20	no	p,d	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
20030	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
20040	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
30060	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
30070	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
40090	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
50100	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
50110	20	yes	p,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
60000	150	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
70140	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
70150	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
80160	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
80170	20	no	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
90190	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
110220	20	no	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
110230	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
120240	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
120250	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
120260	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
130270	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
140280	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
140290	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
140300	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
150310	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
160320	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances

Continued on next page

Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
160330	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
160340	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
160360	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
170350	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
170370	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
180360	20	no	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
180380	20	no	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
180400	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
190390	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
190400	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
190410	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
200400	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
200420	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
200430	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
200440	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
200460	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
200480	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
210450	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
220460	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
220470	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
220480	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
220490	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
220500	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
230000	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
240500	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
240520	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
240530	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
240540	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
250550	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
260540	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
260560	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
260570	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
260580	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
270580	20	no	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
270581	20	no	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
270590	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
280580	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
280590	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
280600	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
280610	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
280620	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
280640	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
290630	150	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
290650	150	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
300000	20	no	p,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
310000	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
320700	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
320720	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
320730	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
320740	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
320760	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
330750	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
340740	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
340760	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
340770	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
340780	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
340790	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
340800	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
340820	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
350790	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
350810	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
360780	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
360800	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
360820	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
360830	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
360840	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
360850	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
360860	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
370850	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
370860	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
370870	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
380840	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
380860	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
380870	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
380880	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
380890	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
380900	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
390890	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
390900	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
390910	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
400900	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
400910	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
400920	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
400930	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
400940	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
400950	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
400960	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
410930	150	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
410940	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
410950	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420920	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420940	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420950	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420960	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420970	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420980	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
420990	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
421000	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
430990	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
440960	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
440980	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
440990	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
441000	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
441010	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
441020	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
441030	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
441040	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
441050	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
441060	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
451030	30	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	?	?
451050	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
461020	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
461040	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
461050	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
461060	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
461070	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
461080	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
461100	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
471070	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
471090	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
471101	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
471110	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
481060	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
481080	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
481100	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
481110	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
481120	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
481130	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
481140	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
481151	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
481160	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
491130	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
491150	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501120	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501140	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501150	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501160	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501170	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501180	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501190	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501200	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501220	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501230	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
501240	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
501250	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
501260	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
511210	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
511230	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
511240	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
511250	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
511260	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
521200	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
521220	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521230	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521240	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521250	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521260	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521271	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
521280	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521291	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
521300	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
521320	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
531270	30	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	?	?
531290	30	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	?	?
531300	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
531310	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
531350	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
541240	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541260	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541280	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541290	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541300	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541310	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541320	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541330	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
541340	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
541350	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
541360	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
551330	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
551340	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
551350	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
551360	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
551370	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561300	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561320	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561340	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561350	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561360	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561370	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
561380	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
561400	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
571380	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
571390	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
571400	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
581400	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
581410	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
581420	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
581430	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
581440	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
591410	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
591420	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
591430	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
601420	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
601430	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
601440	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
601450	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
601460	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
601470	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
601480	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
601500	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
611470	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
611480	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
611481	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
611490	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
611510	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
621440	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
621470	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
621480	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
621490	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
621500	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
621510	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
621520	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
621530	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
621540	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
631510	20	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
631520	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
631530	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
631540	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
631550	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
631560	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
631570	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
641520	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
641540	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
641550	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
641560	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
641570	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
641580	20	no	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
641600	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
651590	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
651600	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
661600	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
661610	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
661620	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
661630	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
661640	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
671650	30	yes	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
681620	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
681640	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
681660	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
681670	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
681680	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
681700	20	yes	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
711750	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
711760	20	no	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
721740	20	yes	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
721760	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
721770	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
721780	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
721790	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
721800	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
731810	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
731820	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
741820	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
741830	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
741840	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
741860	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
751850	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
751870	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	yes	
760000	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
771910	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
771930	20	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	yes	
780000	20	yes	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
791970	30	yes	p,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
801960	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
801980	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
801990	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
802000	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
802010	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
802020	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
802040	20	yes	p,d,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
810000	20	no	p,d,t,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
822040	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
822060	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
822070	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
822080	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
832090	200	yes	p,d,t,^{3}He,α	no	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
882230	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
882240	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
882250	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
882260	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
892250	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
892260	20	no	-	no	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
892270	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no resonances

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
902270	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	no	no resonances
902280	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
902290	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
902300	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
902320	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
902330	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
902340	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
912310	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
912320	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
912330	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	yes	
922320	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
922330	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
922340	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
922350	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
922360	30	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
922370	30	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
922380	30	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
932350	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
932360	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
932370	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
932380	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
932390	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	no	no resonances
942360	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
942370	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
942380	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
942390	30	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
942400	30	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
942410	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
942420	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
942430	20	yes	-	total	no	300, 600, 900, 1200, 1500, 1800	yes	
942440	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	yes	
942460	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
952410	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
952420	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
952421	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
952430	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
952440	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
952441	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
962400	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
962410	20	no	-	total	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
962420	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
962430	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
962440	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
962450	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
962460	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
962470	20	yes	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
962480	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
962490	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
962500	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
972470	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no unresolved resonances
972490	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
972500	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
982490	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
982500	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	yes	
982510	20	yes	-	both	yes	300, 600, 900, 1200, 1500, 1800	yes	
982520	20	yes	-	total	no	300, 600, 900, 1200, 1500, 1800	no	negative values in ptable
982540	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
992530	-	-	-	-	-	-	-	-

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Nuclide	E_{max}	GPD	CP	$\bar{\nu}$	DN	T [K]	Probability tables	
992540	20	no	-	both	yes	300, 600, 900, 1200, 1500, 1800	no	no resonances
992550	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances
1002550	20	no	-	both	no	300, 600, 900, 1200, 1500, 1800	no	no resonances

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