Nuclear data, uncertainties and their applications

Part 2: adjustment of nuclear data

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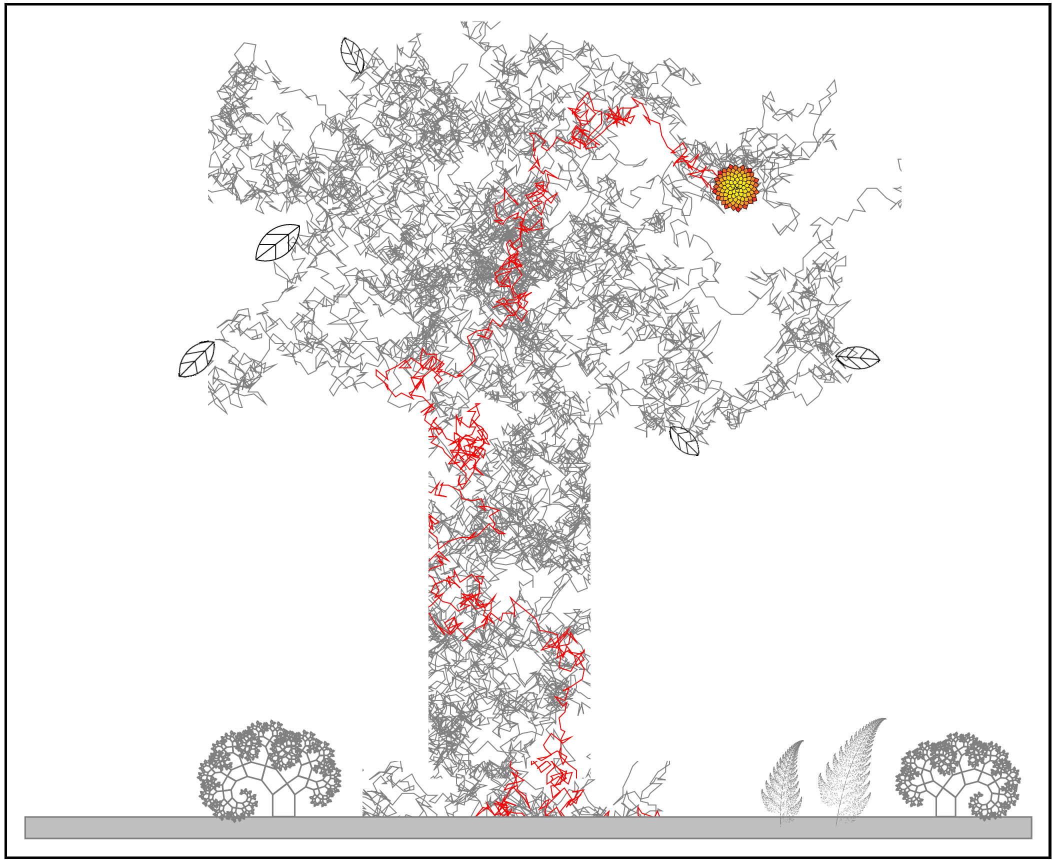


All slides can be found at:
ftp://ftp.nrg.eu/pub/www/talys/bib_rochman/presentation.html).

Optimum
Search and find
(the Petten method)

- Started in 2010
- Two publications so far
- Controversial (if understood at all)
- We believe this is the future of nuclear data evaluation work
- It might be the only way to sensibly improve C/E

The Petten method on ^{239}Pu

Total Monte Carlo + selection

$$\Longrightarrow \frac{1}{TMC}$$

① Use TALYS to create a single ^{239}Pu evaluation close or equal to ENDF/B-VII.0 or JEFF-3.1.1

② Randomize all model parameters (resonances, nubar, fission neutron spectrum, TALYS parameters) to create 500 random ^{239}Pu evaluations

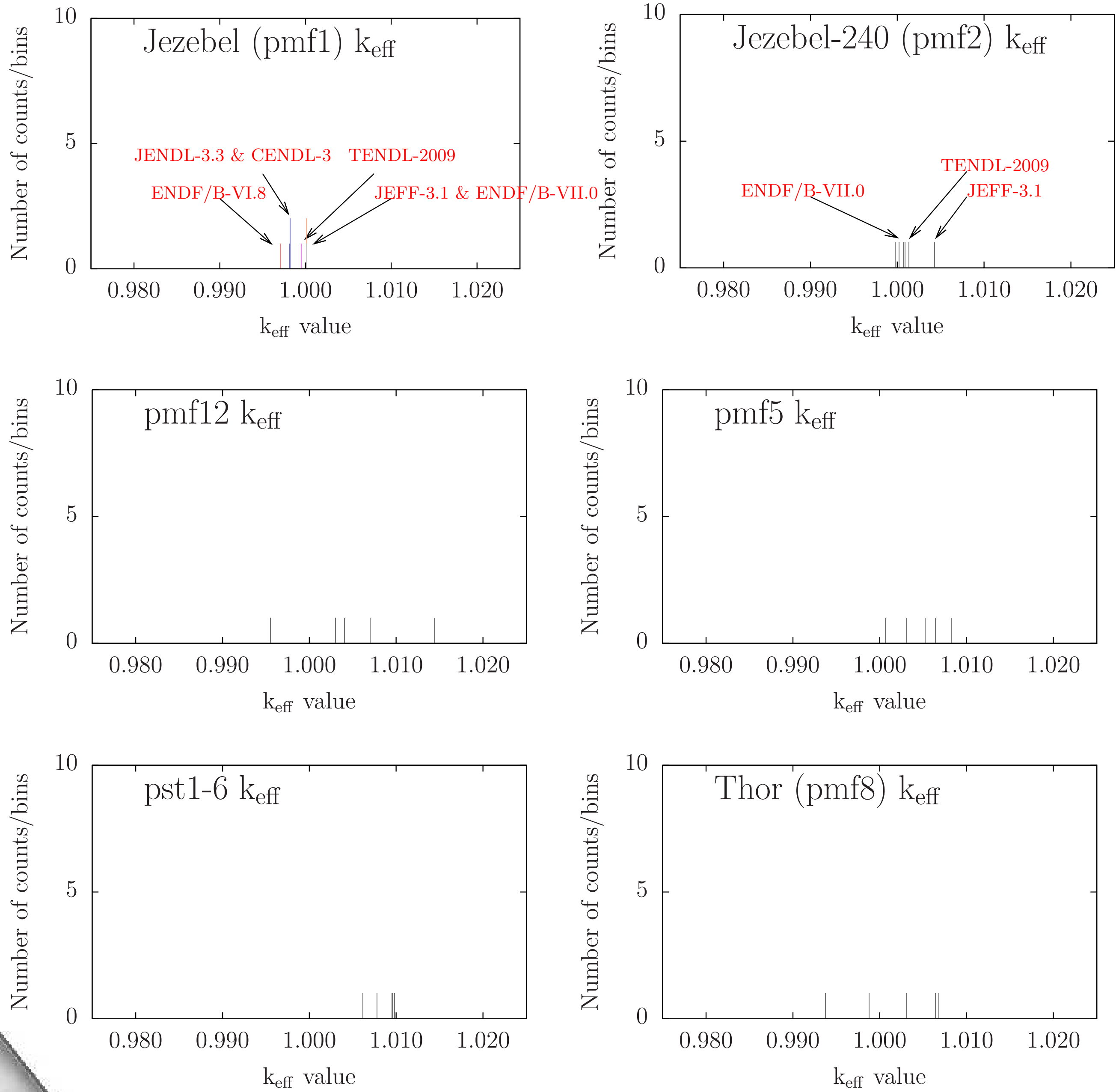
③ Benchmarks the $n \geq 500$ files with the same set of criticality benchmarks

④ Select the best random file

Example: 100 benchmarks, 500 random files $\Longrightarrow$ 500 TALYS + NJOY and $100 \times 500 = 5 \cdot 10^4$ MCNP loops,

1.4 years on a single processor, or 5 days on 100 processors (3 GHz)

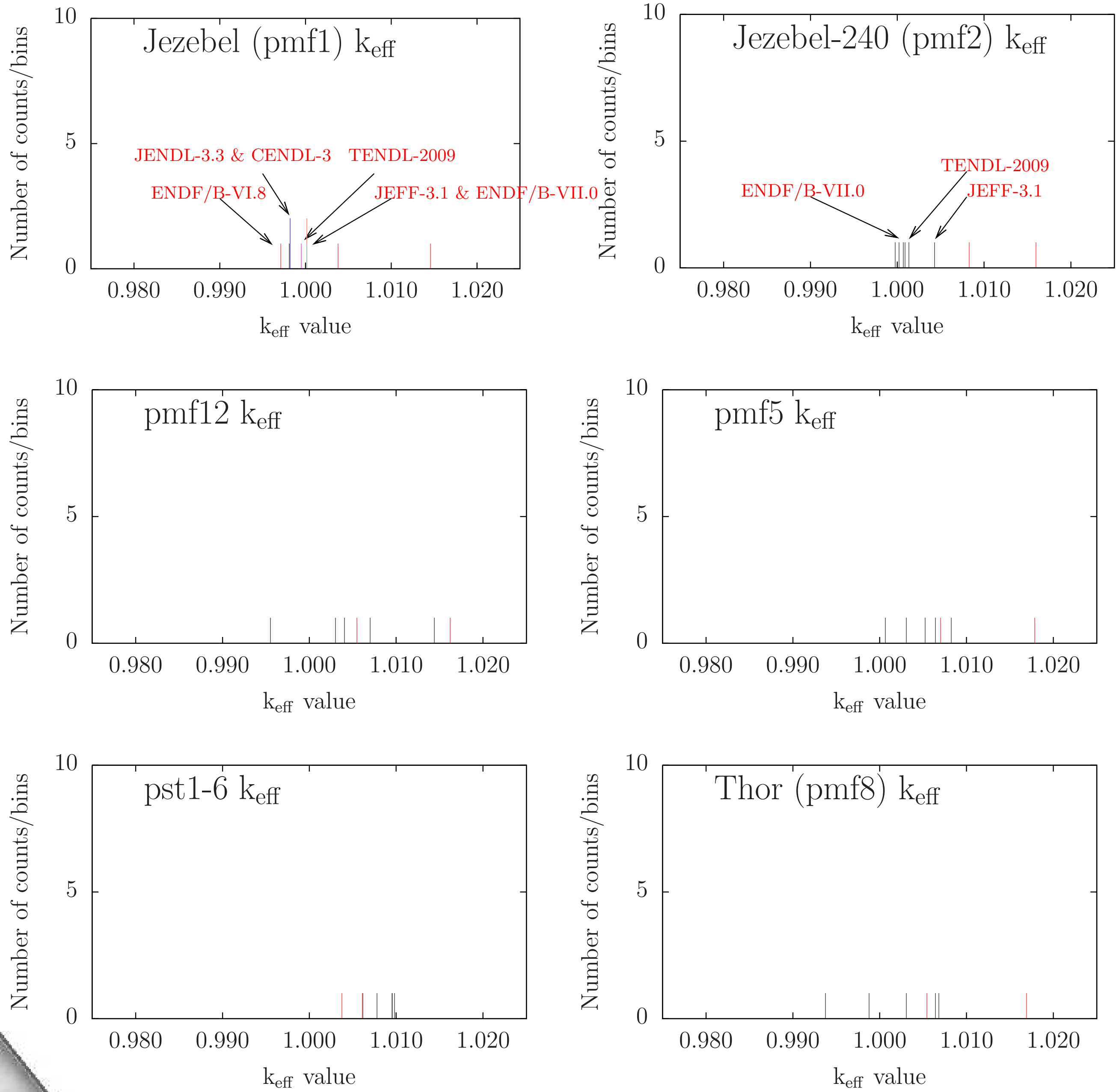
The Petten method: simple example with 6 k_{eff} benchmarks



	α
JEFF-3.1.1:	$1.14e^{-4}$
JENDL-3.3:	$1.71e^{-4}$
TENDL-2009:	$3.66e^{-4}$
ENDF/B-VI.8:	$1.72e^{-4}$
ENDF/B-VII.0:	$1.69e^{-4}$

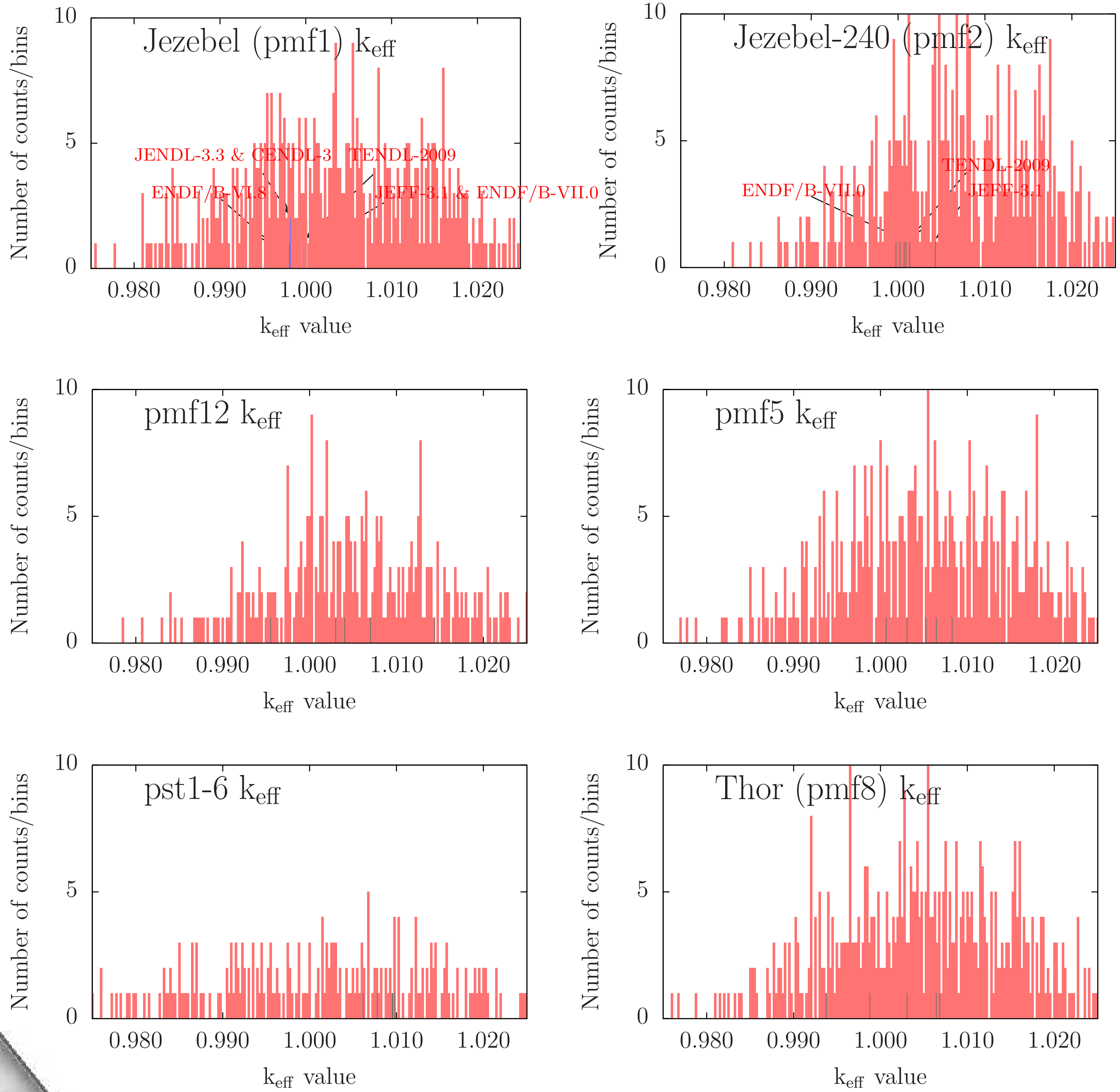
$$\alpha = \sum_{i=0}^{n} \frac{(C_i - E_i)^2}{C_i},$$

The Petten method: simple example with 6 k_{eff} benchmarks

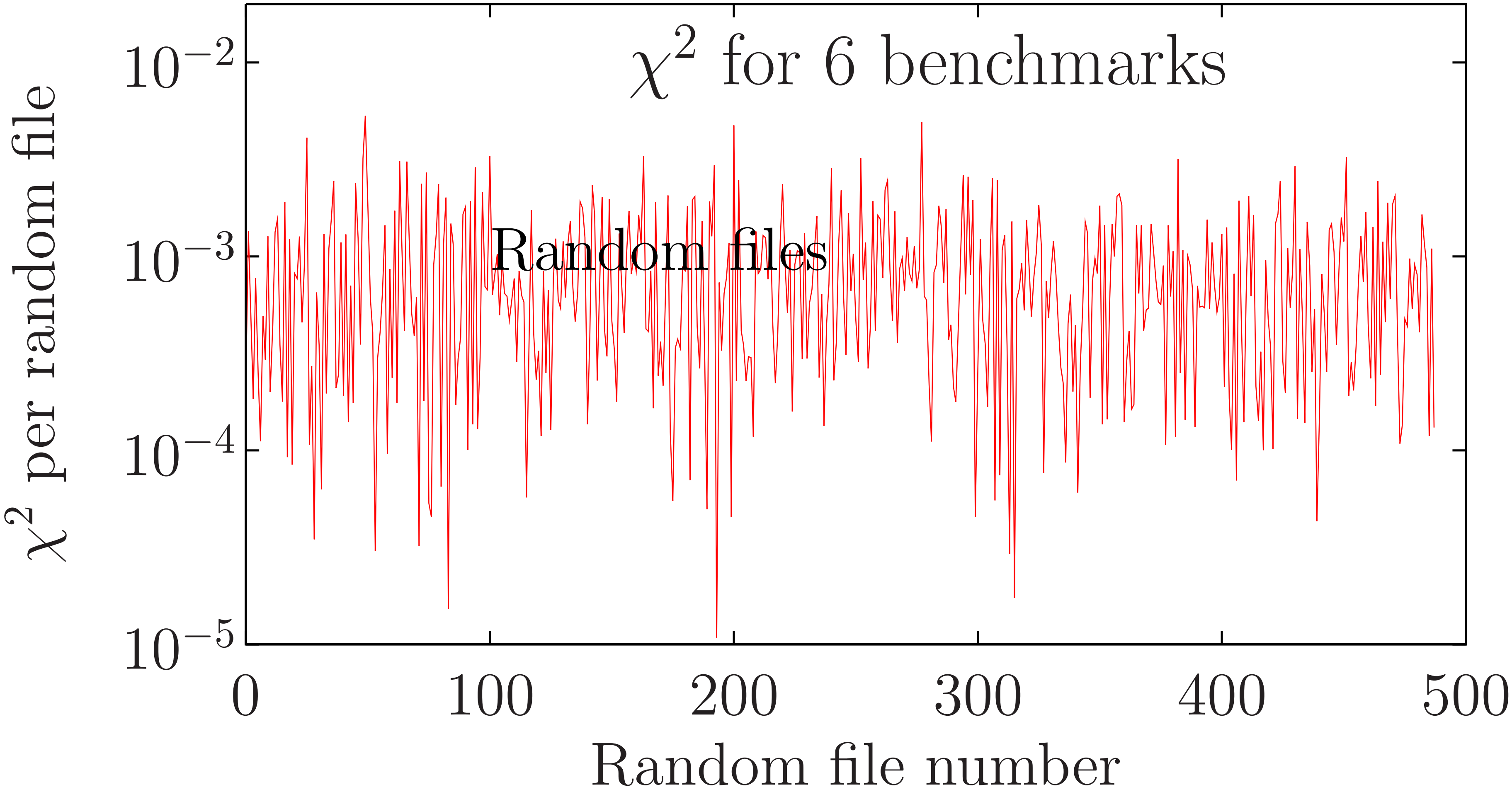


	α
JEFF-3.1.1:	$1.14e^{-4}$
JENDL-3.3:	$1.71e^{-4}$
TENDL-2009:	$3.66e^{-4}$
ENDF/B-VI.8:	$1.72e^{-4}$
ENDF/B-VII.0:	$1.69e^{-4}$
random 0:	$2.29e^{-4}$
random 1:	$13.4e^{-4}$

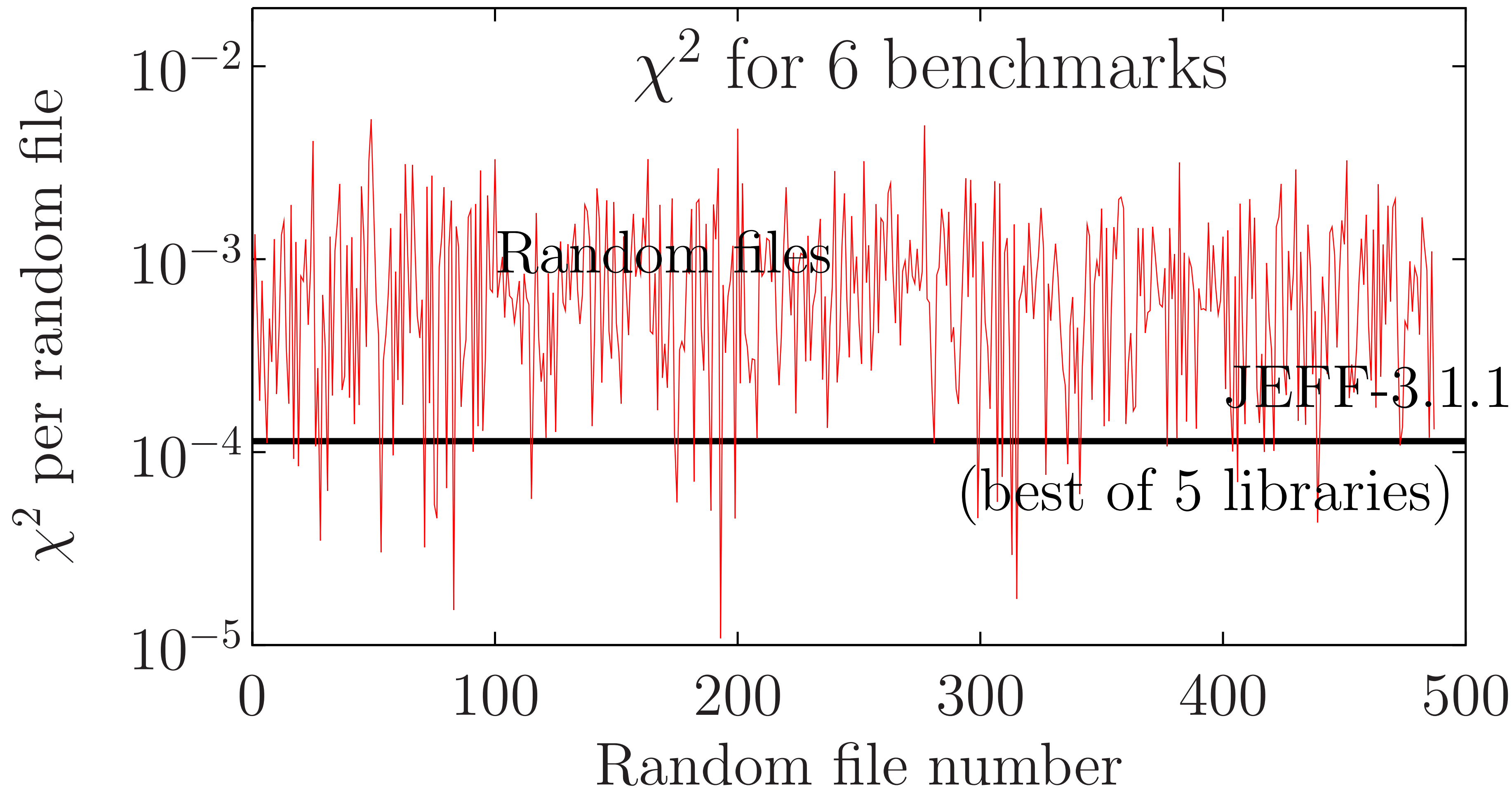
The Petten method:: 6 k_{eff} benchmarks with random ^{239}Pu



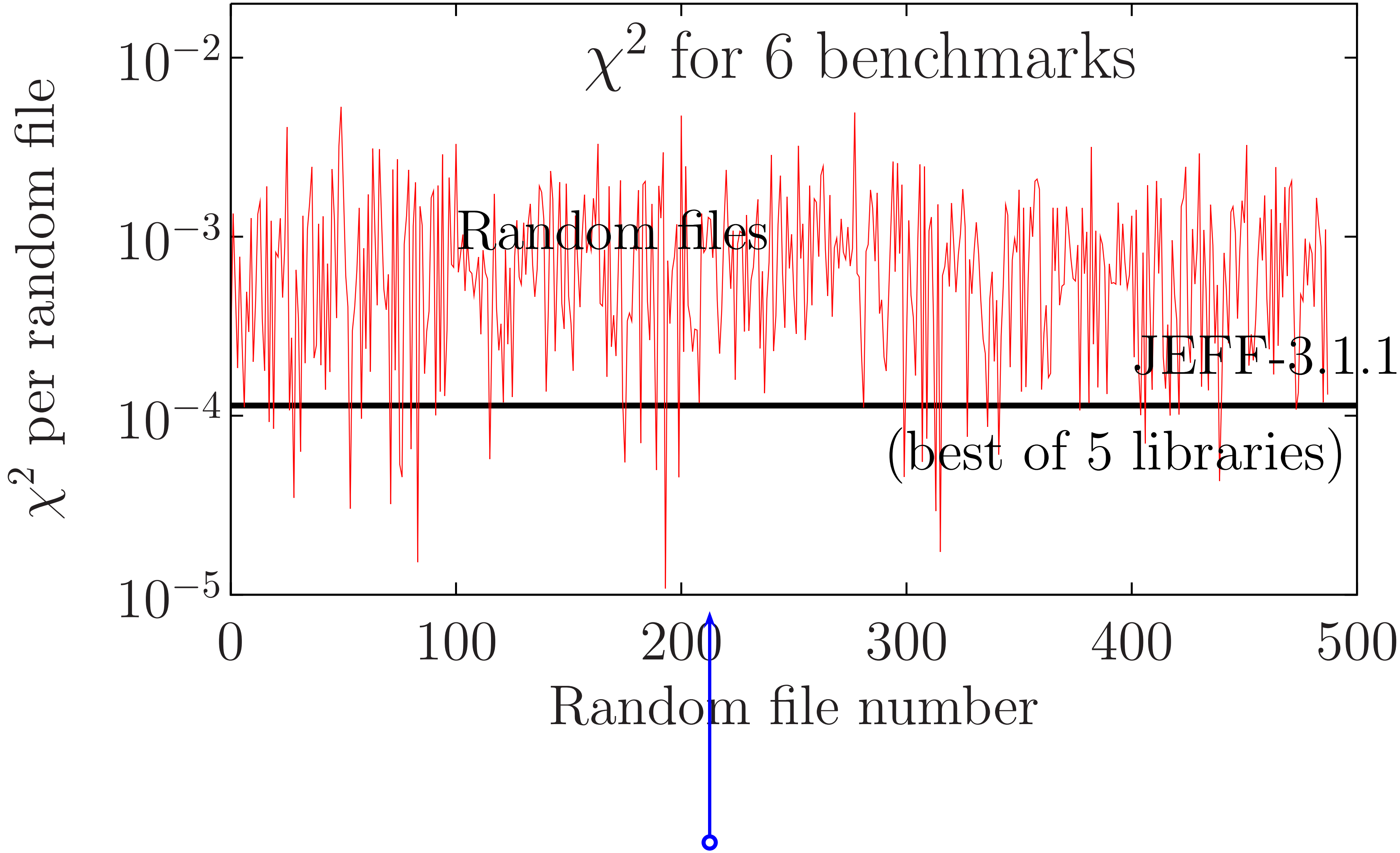
Benchmarking: 6 k_{eff} benchmarks with random ^{239}Pu



Benchmarking: 6 k_{eff} benchmarks with random ^{239}Pu

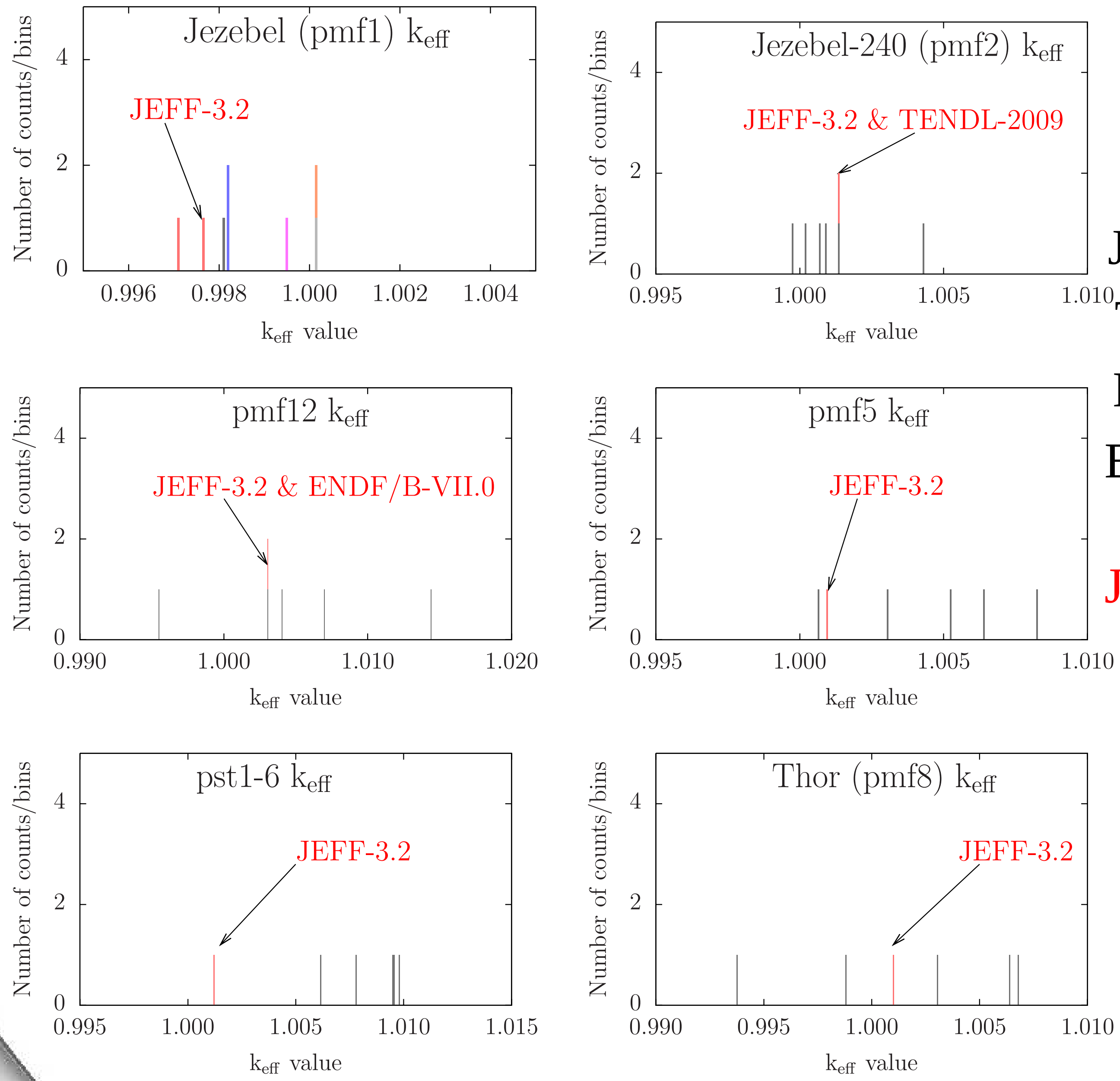


Benchmarking: 6 k_{eff} benchmarks with random ^{239}Pu



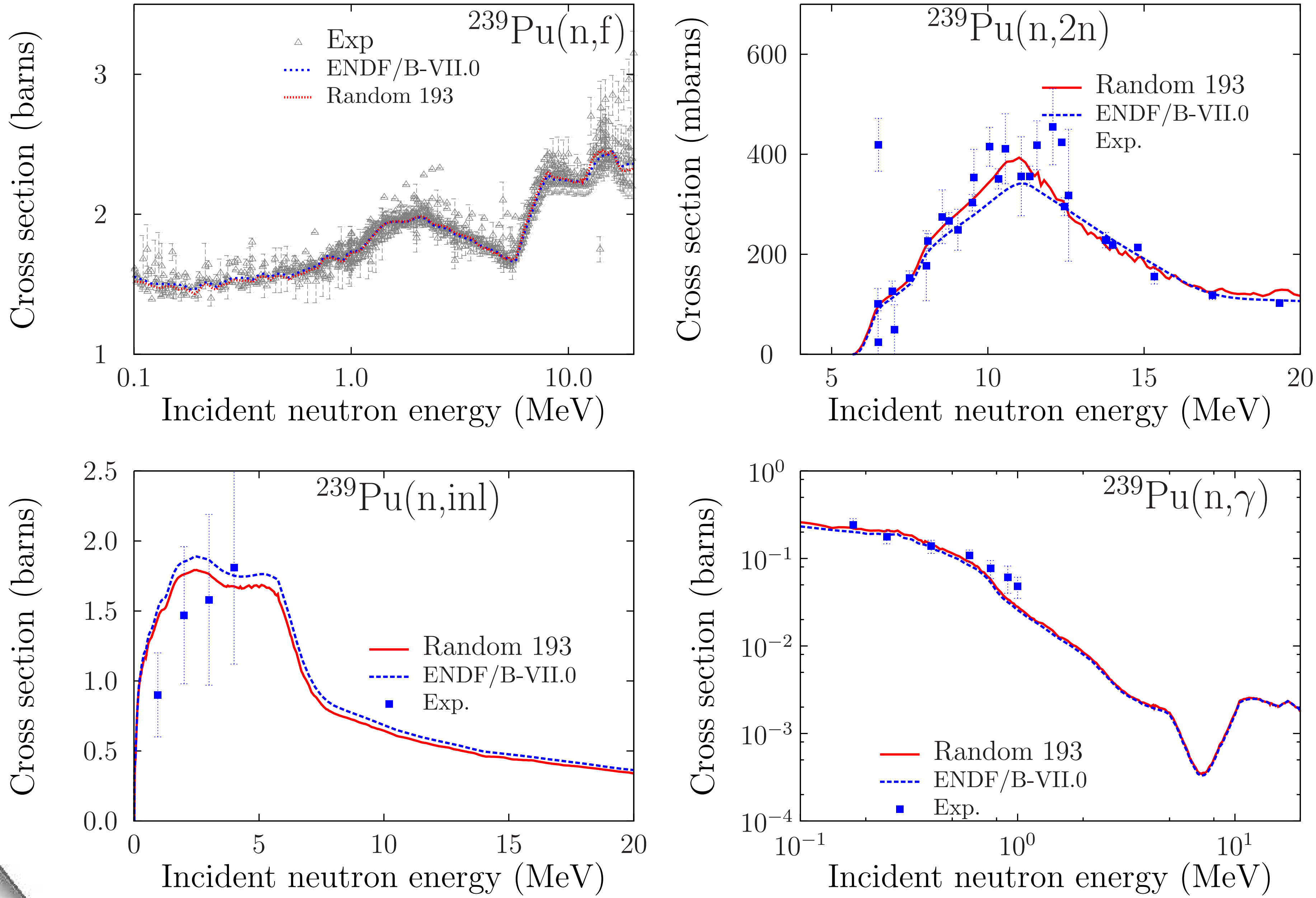
Best χ^2 for random file 193 ($\chi^2 = 1.08e^{-5}$, 10 $\times$ smaller than JEFF-3.1.1, 17 $\times$ smaller than ENDF/B-VII.0)

Benchmarking: 6 k_{eff} benchmarks with random ^{239}Pu

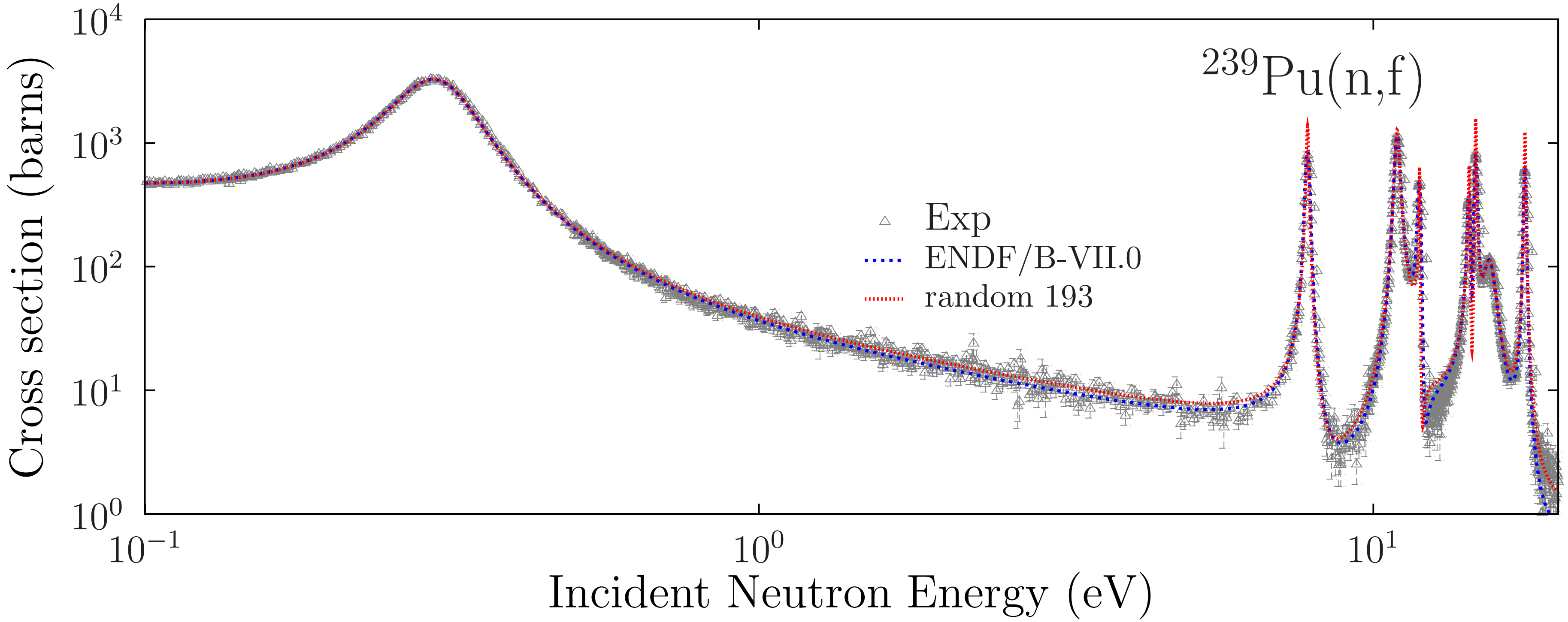


	χ^2
JEFF-3.1:	$1.14e^{-4}$
JENDL-3.3:	$1.71e^{-4}$
TENDL-2009:	$3.66e^{-4}$
ENDF/B-VI.8:	$1.72e^{-4}$
ENDF/B-VII.0:	$1.69e^{-4}$
JEFF-3.2β:	$1.08e^{-5}$

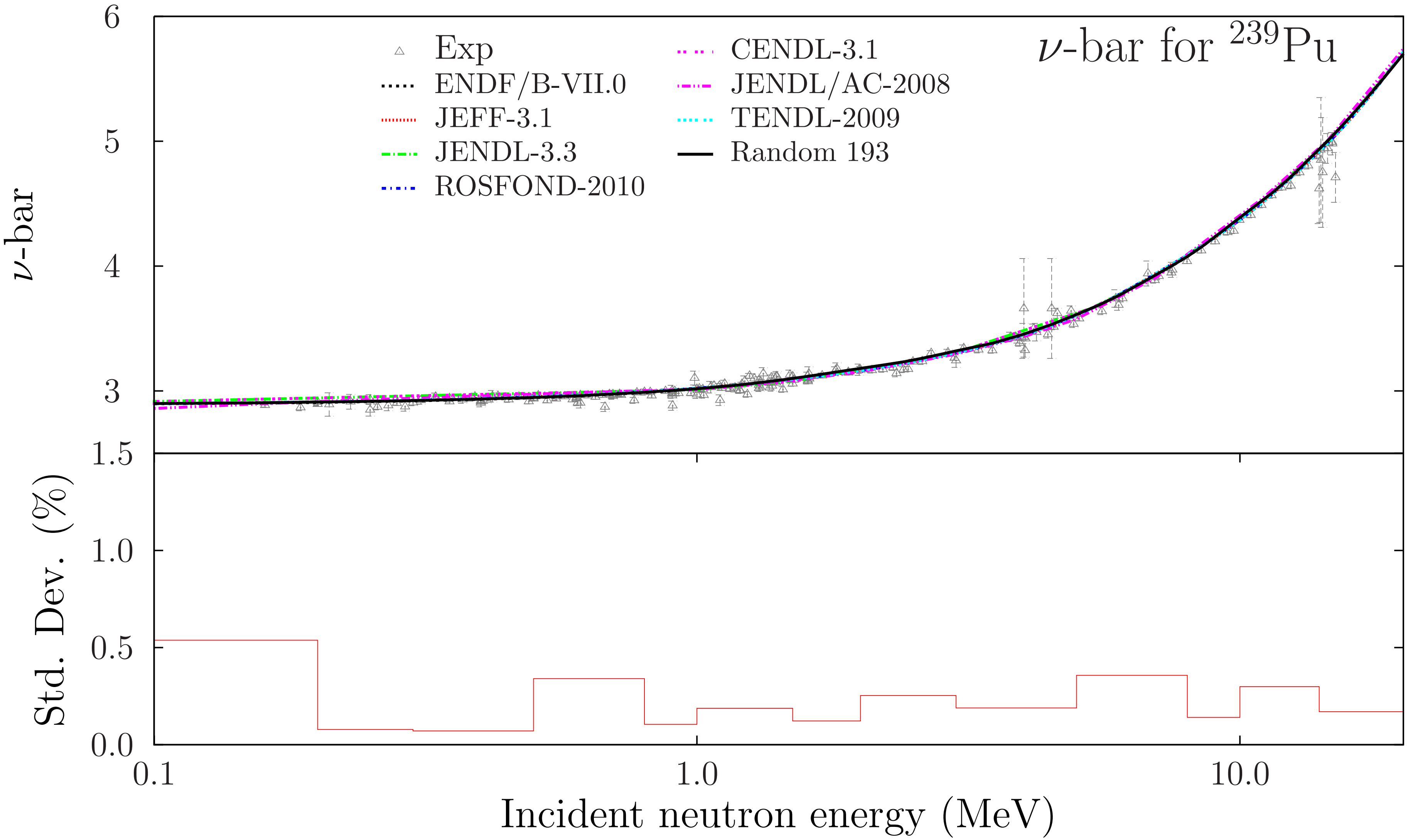
Optimal cross sections (random file 193)



Optimal cross section (random file 193)



Optimal nu-bar (random file 193)



Petten method: real case with 120 ^{239}Pu benchmarks

Table 1: List of plutonium benchmarks selected for the random search.

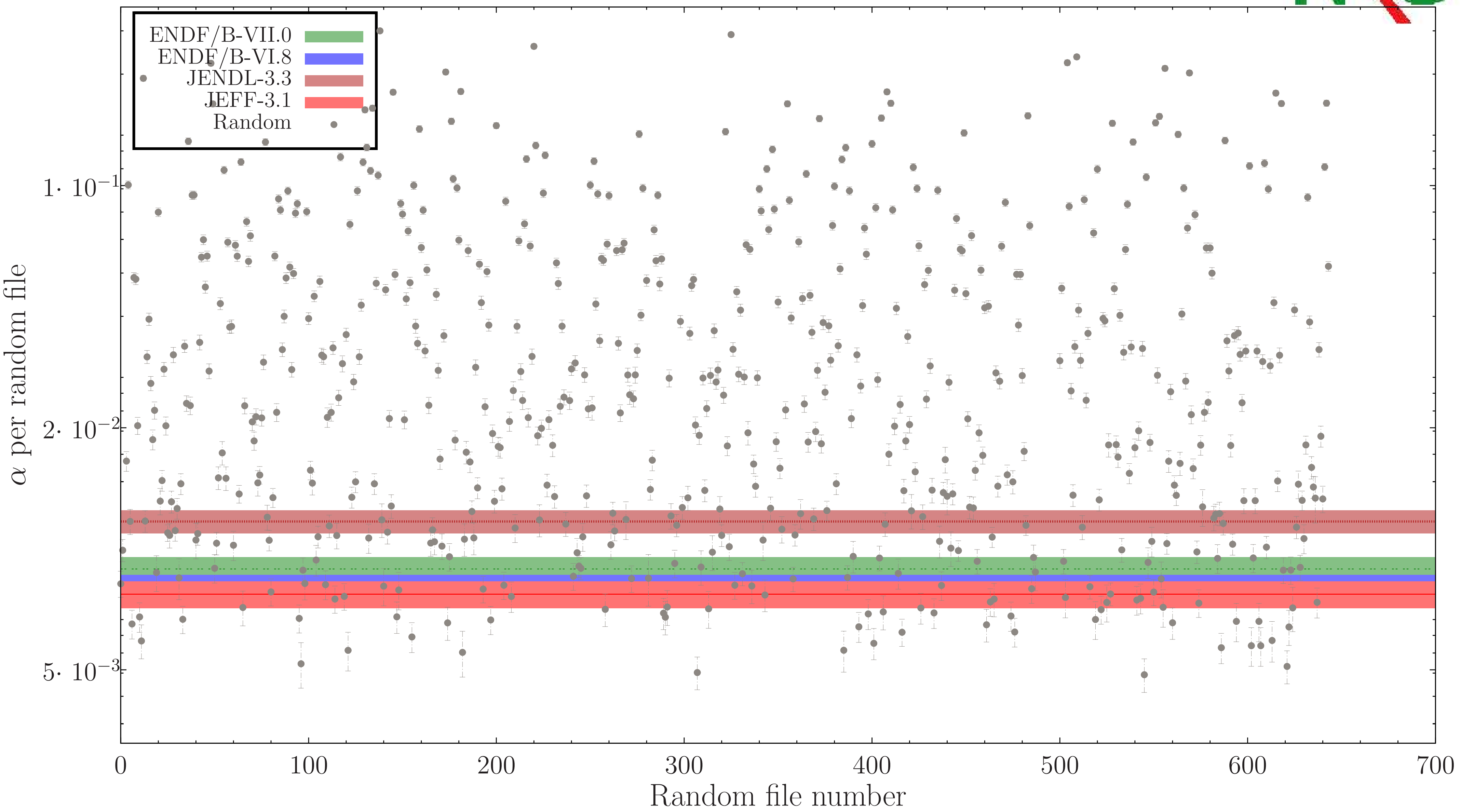
Name	Cases	Name	Cases	Name	Cases	Name	Cases
pmf1	1	pmf2	1	pmf5	1	pmf6	1
pmf8	1	pmf12	1	pmf13	1	pci1	1
pmi2	1	pst1	6	pst2	6	pst3	8
pst4	13	pst5	9	pst6	3	pst7	9
pst8	29	pst12	22	pmm1	6		

$$\chi^2 = \sum_{i=0}^{n} \frac{(C_i - E_i)^2}{C_i}, \tag{1}$$

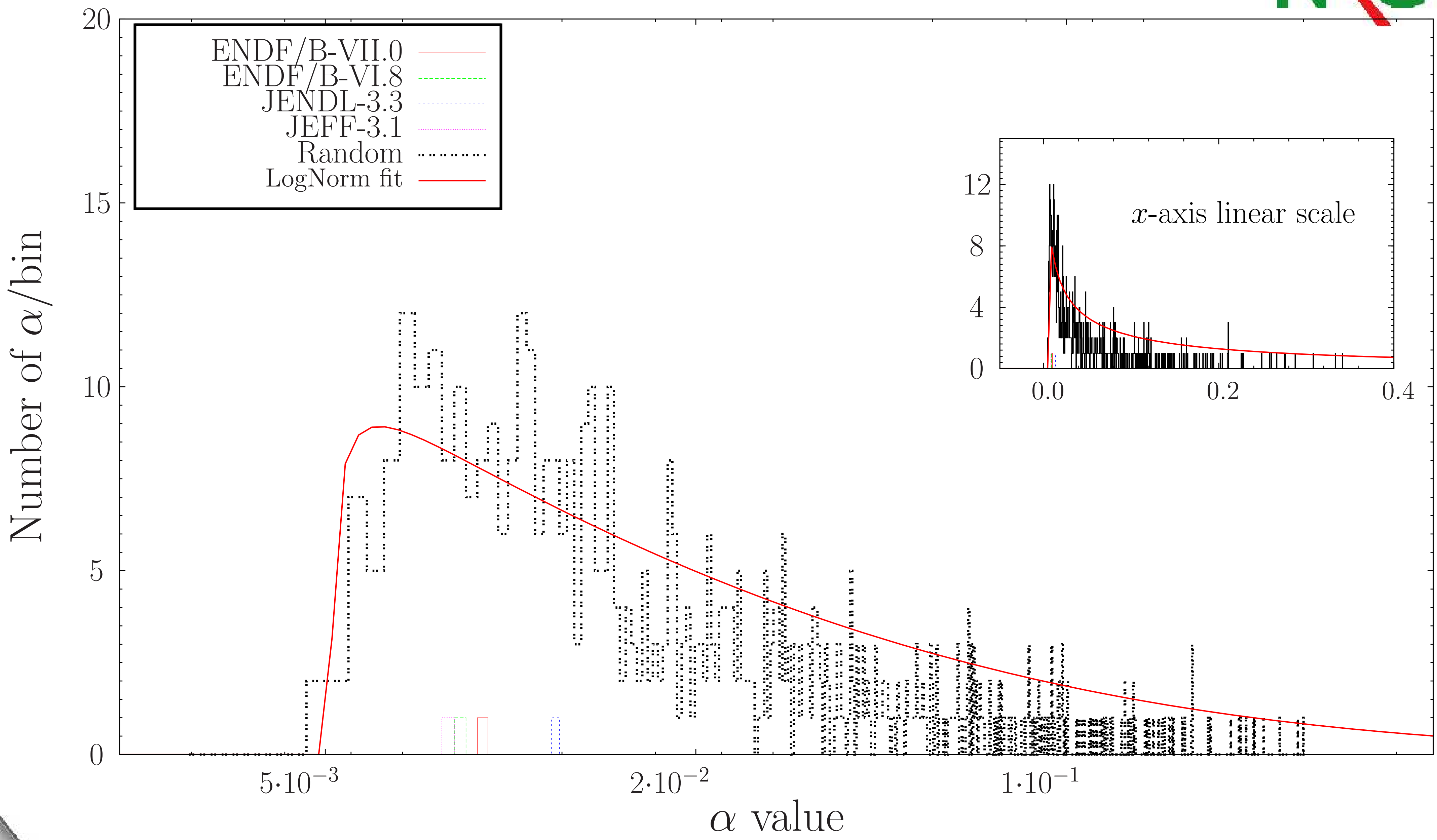
Results independent of the type of factor α, χ^2... or

$$F = 1 - 10^{\sqrt{\frac{1}{N}\sum(\log(E_i) - \log(C_i))^2}} \tag{2}$$

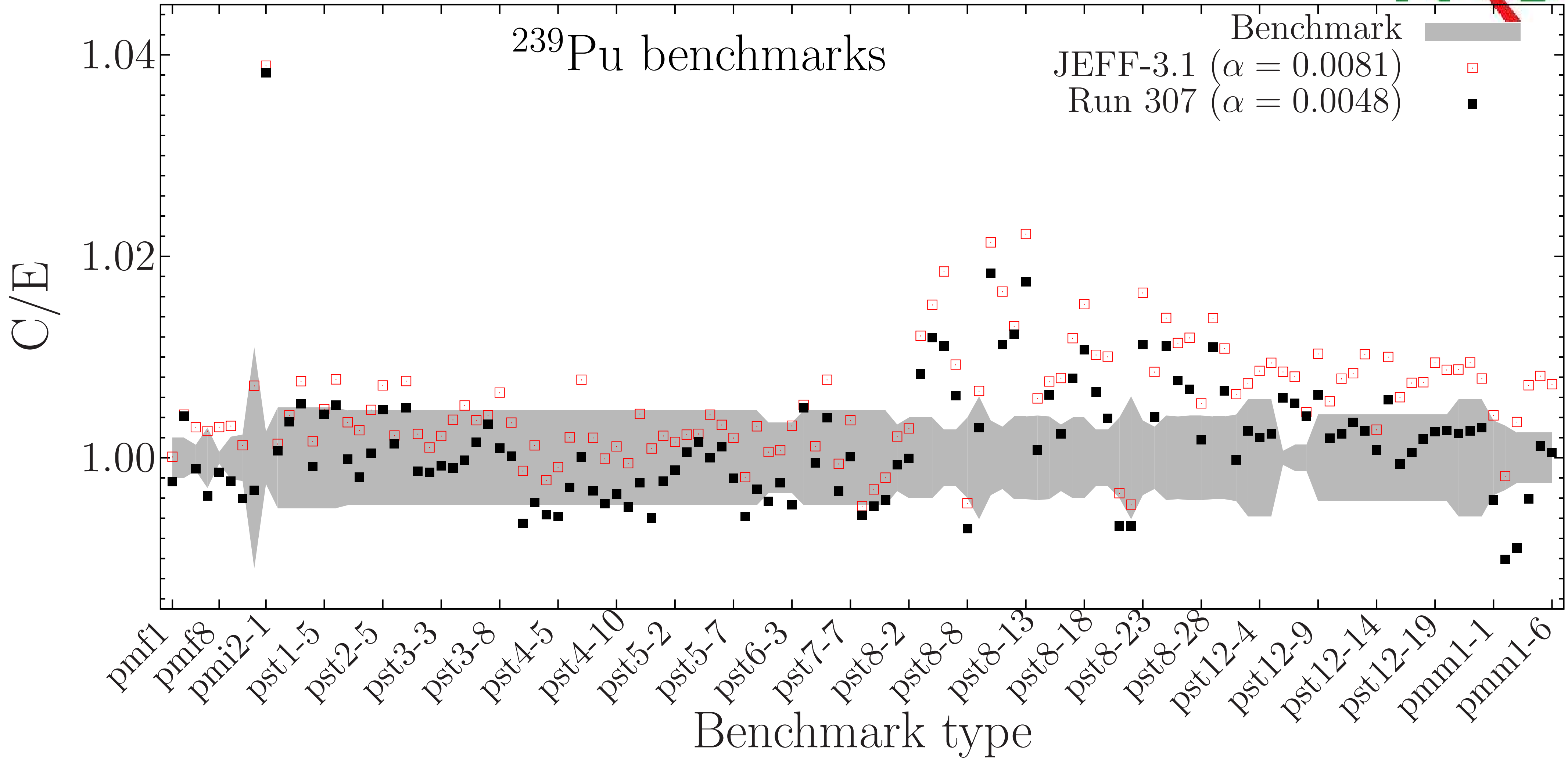
(2) χ^2 values for random ^{239}Pu evaluations



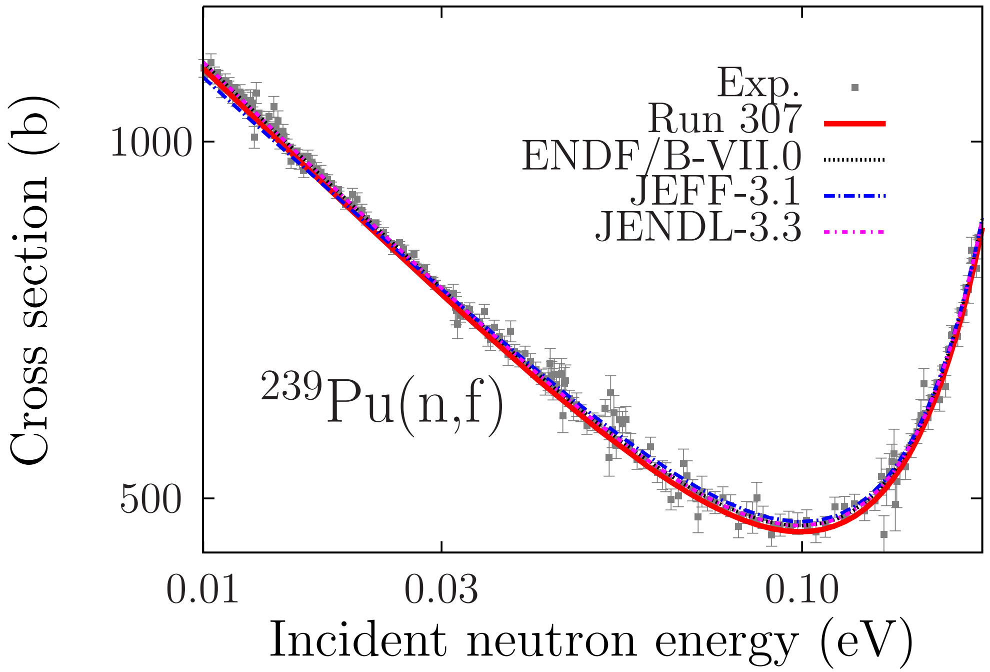
(2) χ^2 values for random ^{239}Pu evaluations

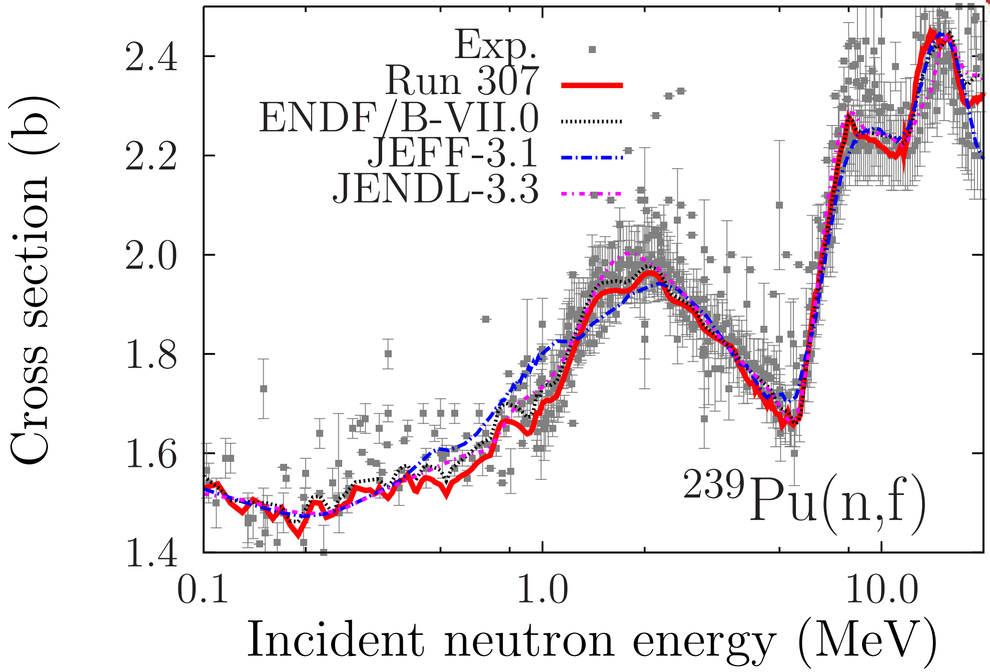


(2) χ^2 values for random ^{239}Pu evaluations



(2) Best ^{239}Pu for this set of benchmarks





Does it work ?

① We have shown that it is possible to "*improve*" an existing evaluation

② Many questions need to be addressed such as

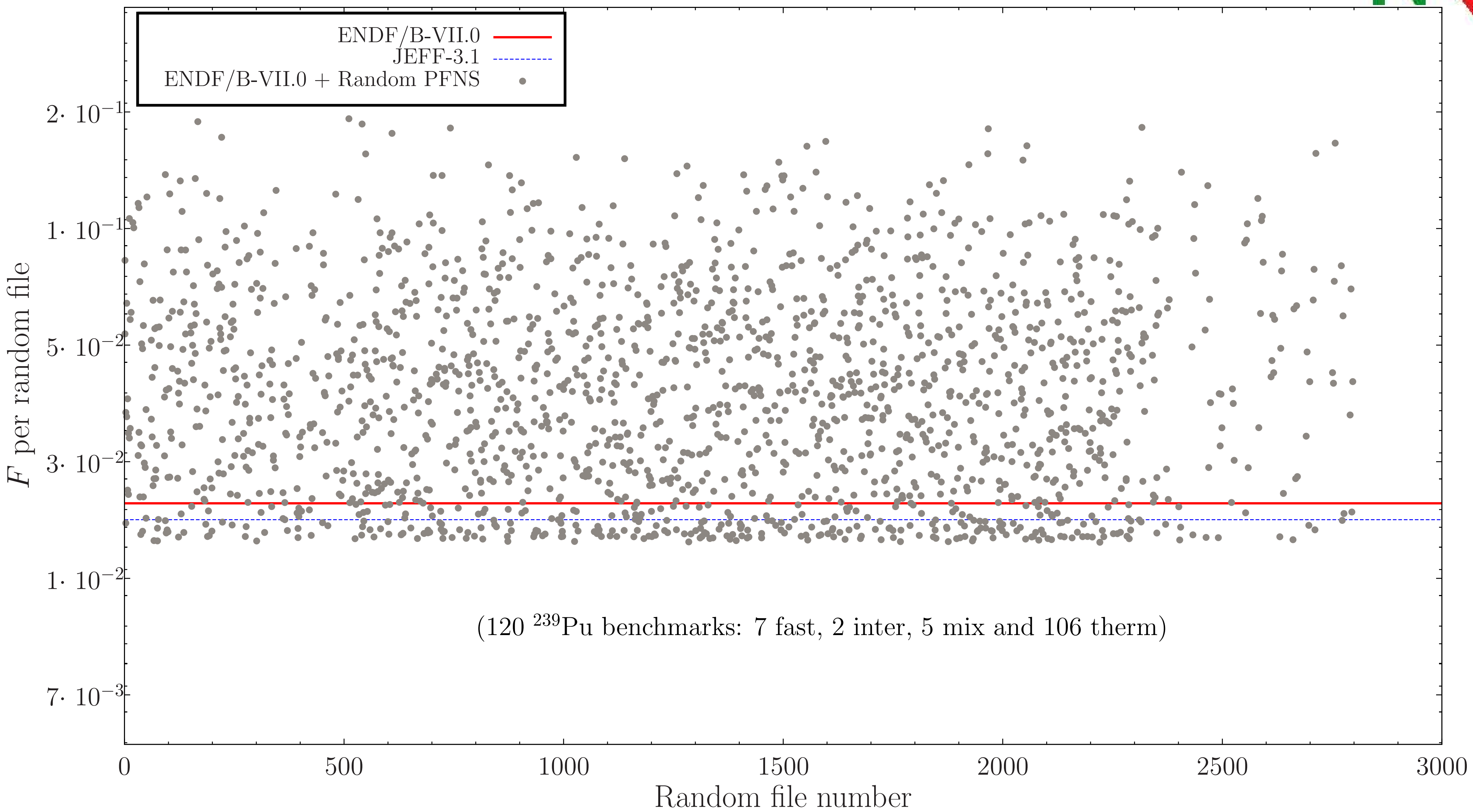
- ➡ Compensation
- ➡ Uncertainty ranges
- ➡ Benchmark list

③ 2^{nd} example: fission neutron spectrum for ENDF/B-VII.0 ^{239}Pu (pfns)

Total Monte Carlo *on pfns*+ selection
$\Longrightarrow$ adjustment *of pfns*

(same benchmarks, keep ENDF/B-VII.0 constant except the pfns, MF5 MT18)

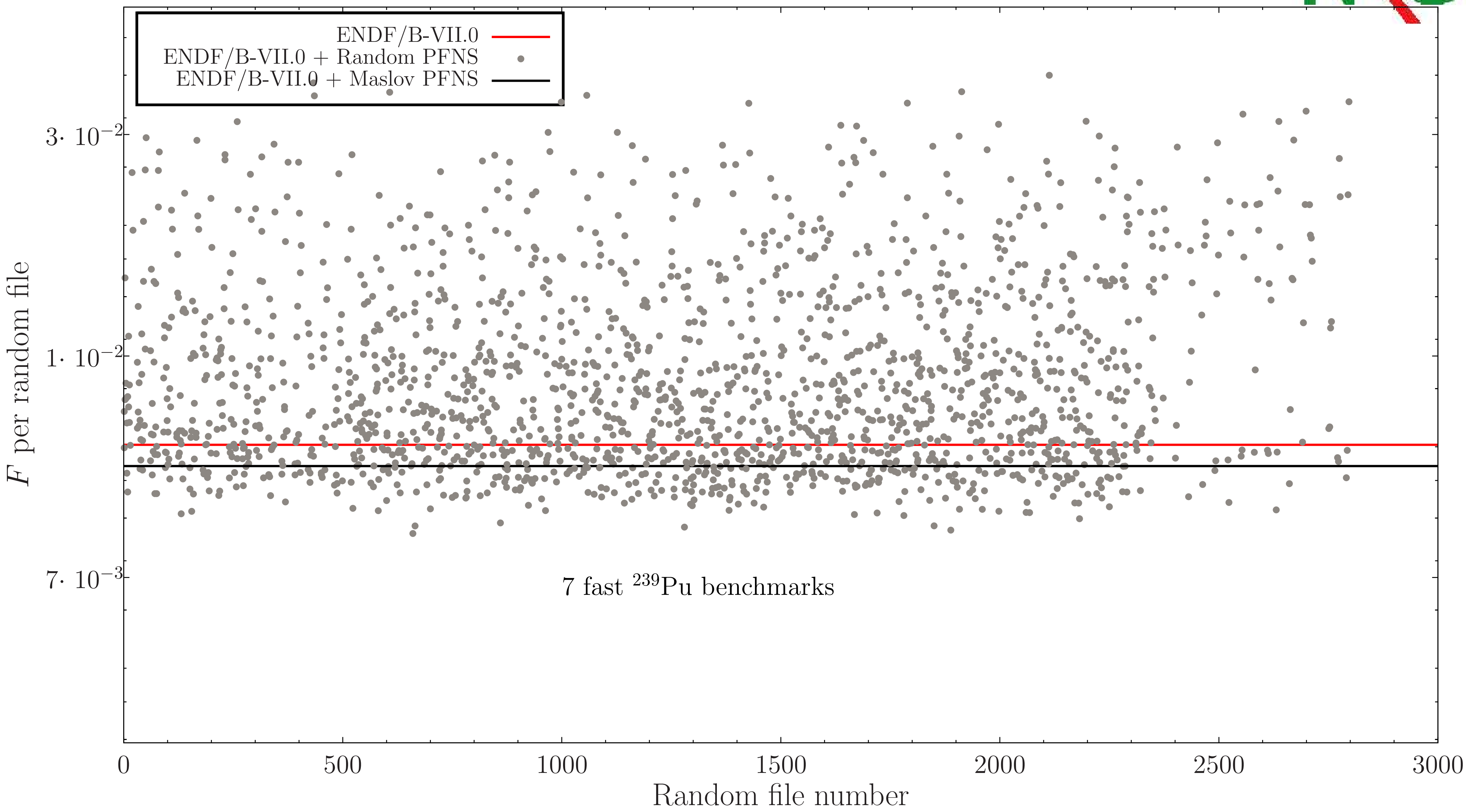
Example 2 on pfns of ^{239}Pu



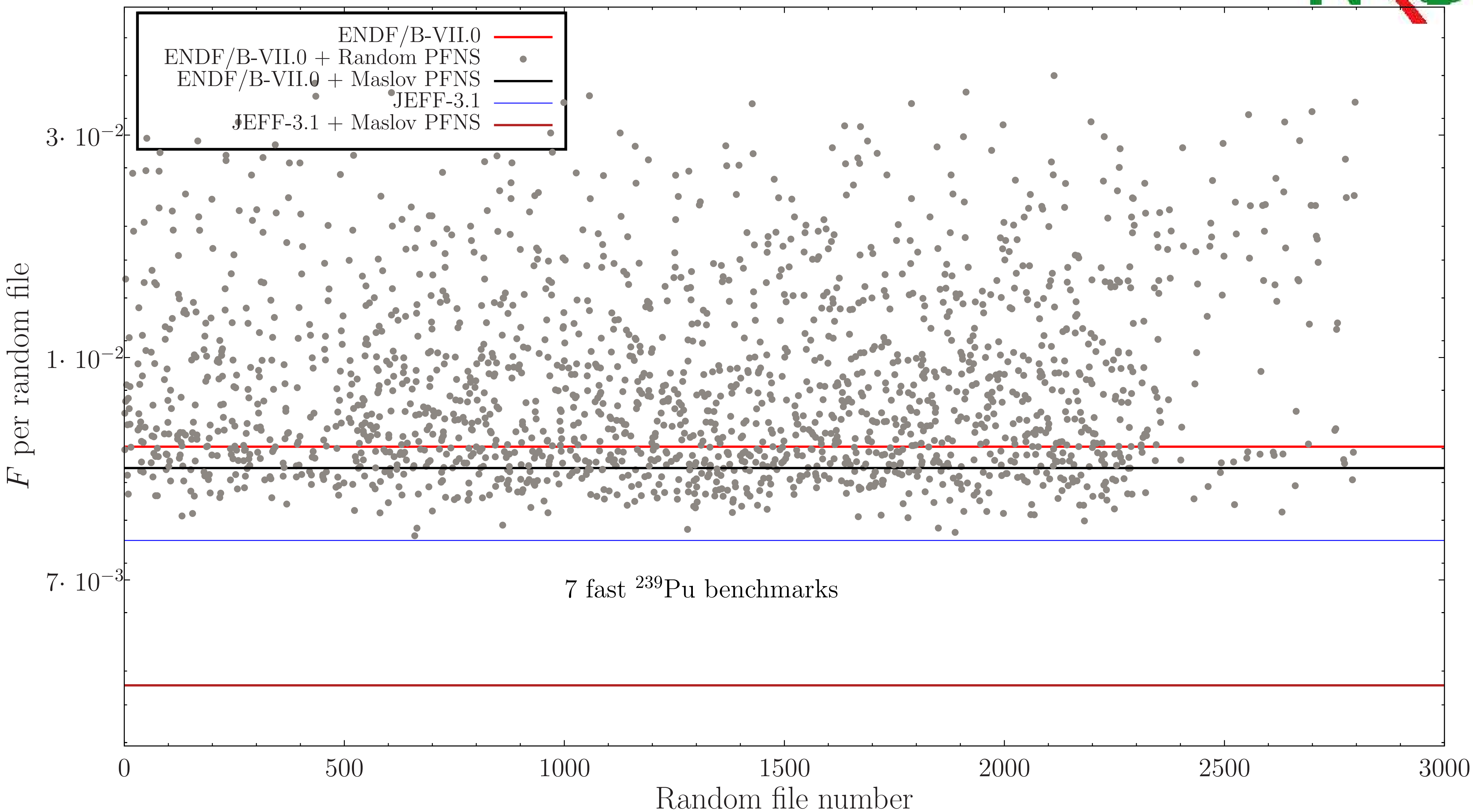
Difference with the previous example (where the whole ^{239}Pu was random): there is a limit in low F

$\Longrightarrow$ like hitting a wall !

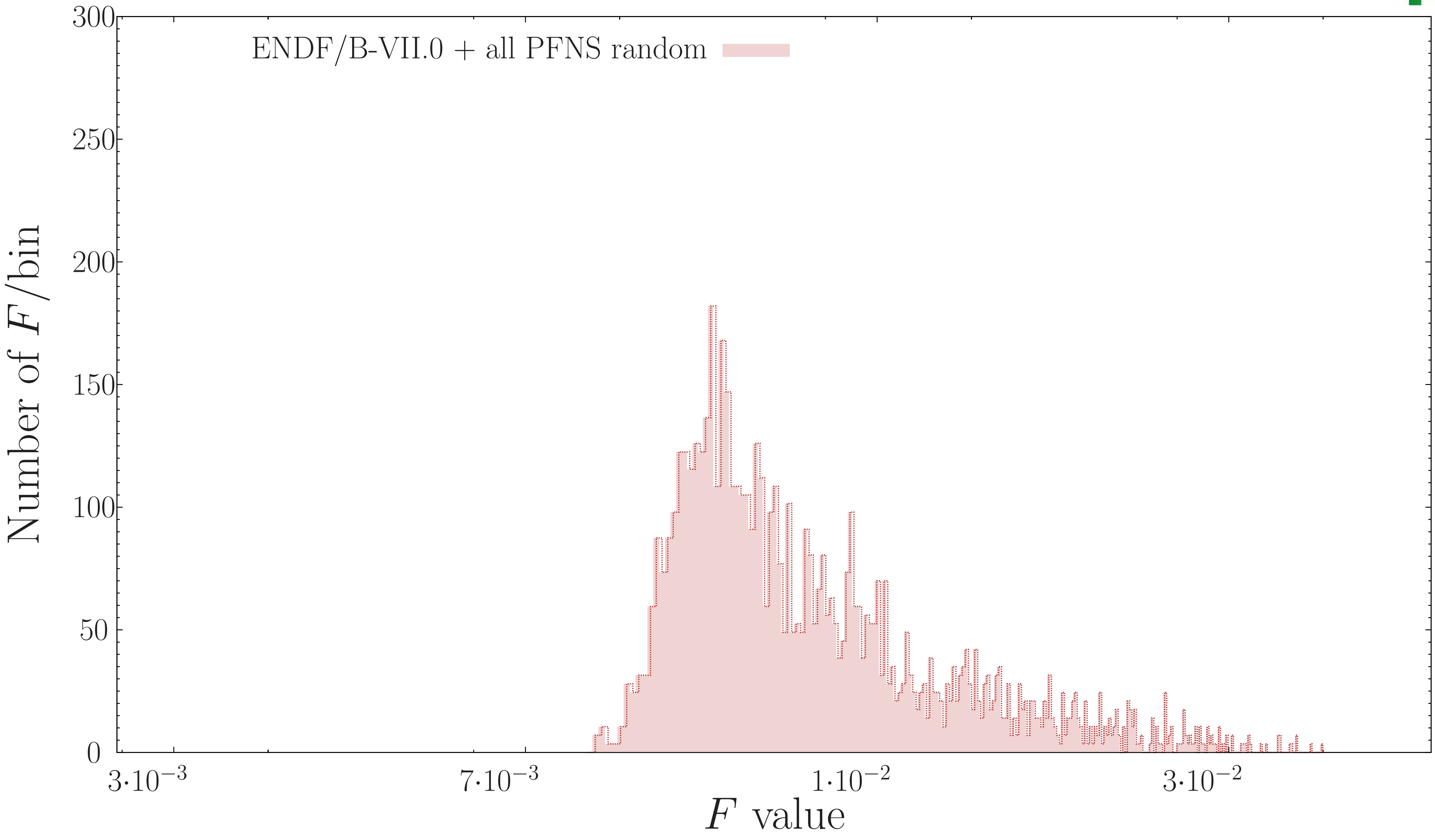
F values for random PFNS ^{239}Pu evaluations



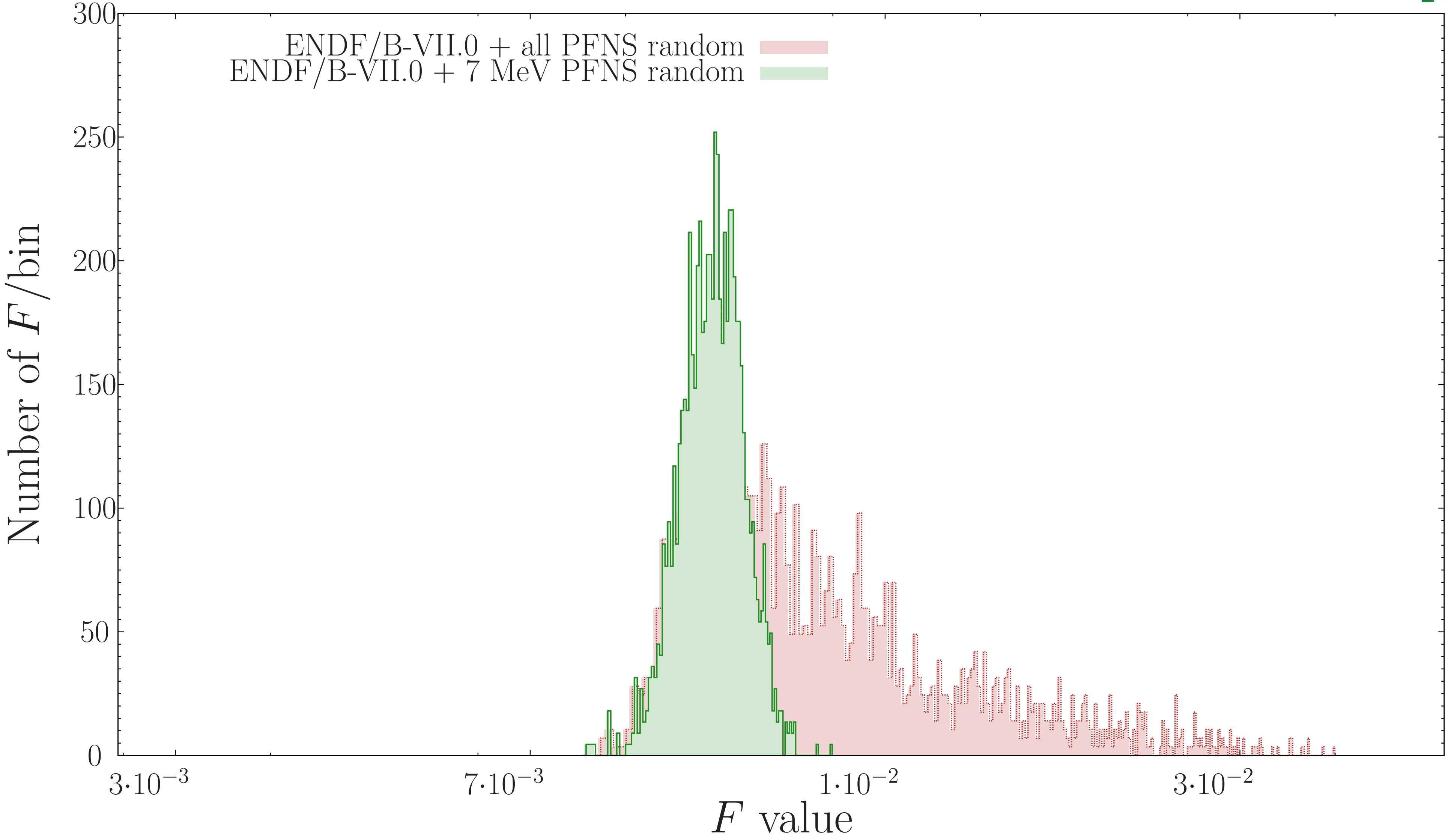
F values for random PFNS ^{239}Pu evaluations



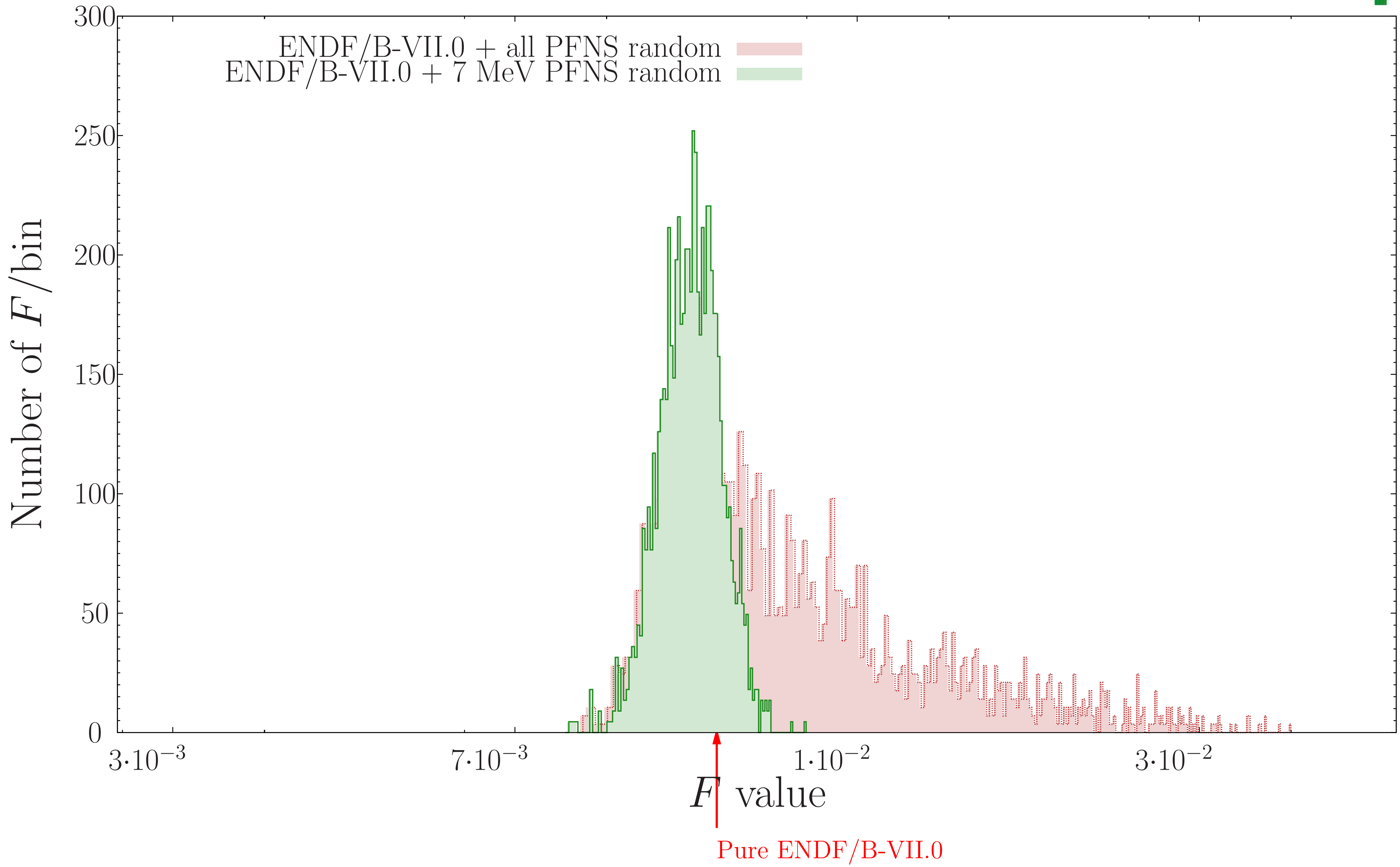
Example 2 on pfns of ^{239}Pu with only 7 fast benchmarks



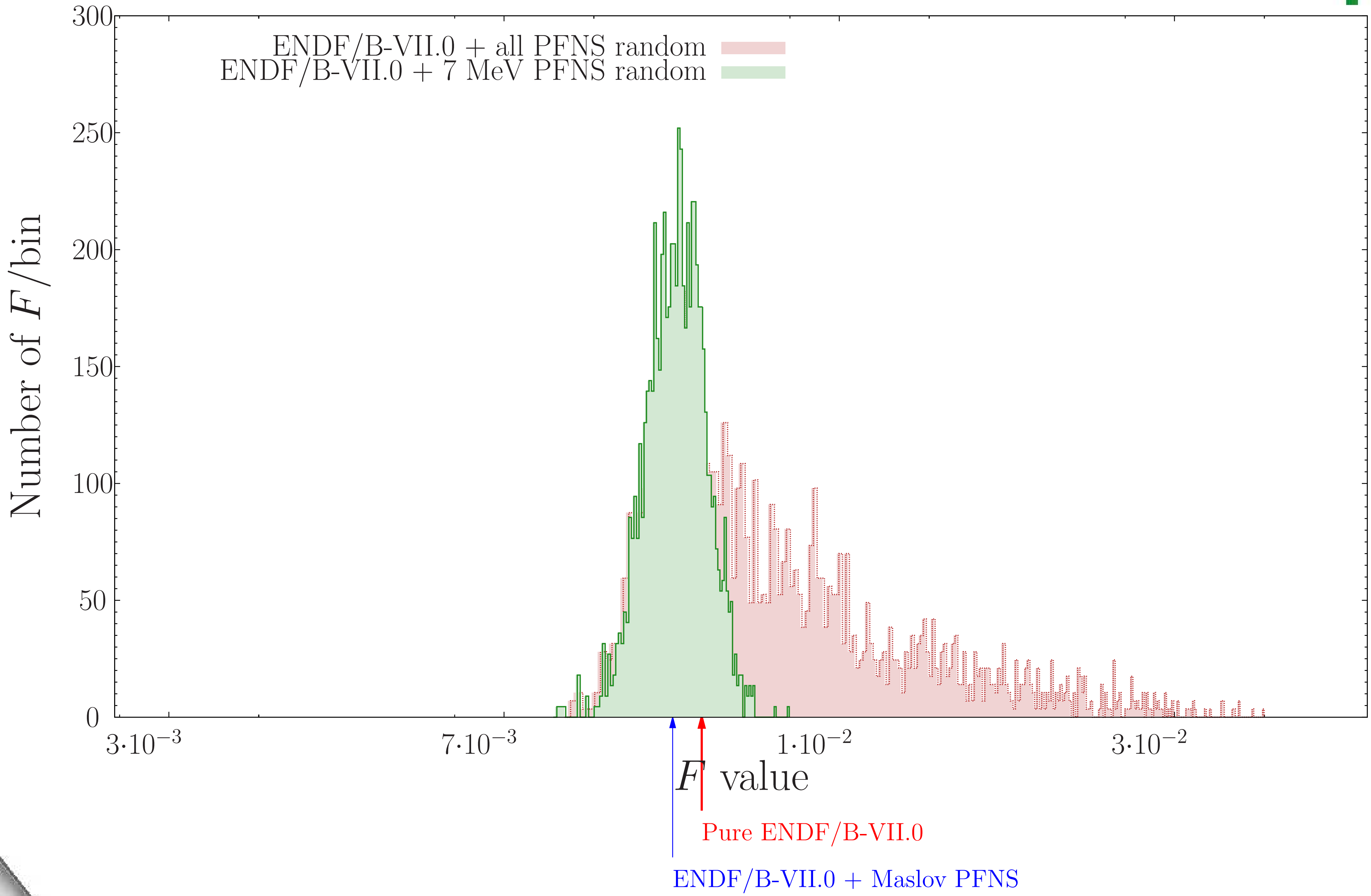
Example 2 on pfns of ^{239}Pu with only 7 fast benchmarks



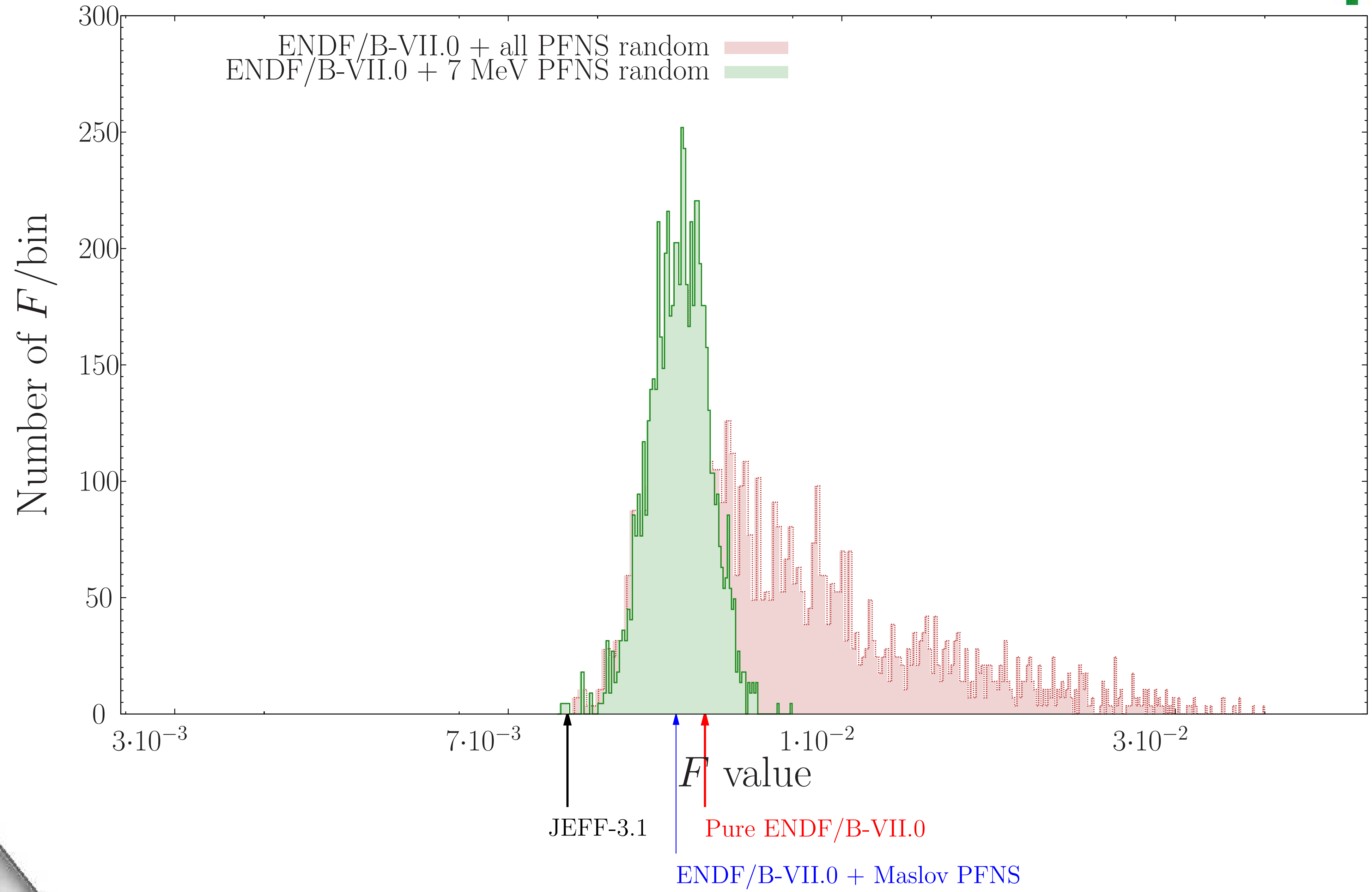
Example 2 on pfns of ^{239}Pu with only 7 fast benchmarks



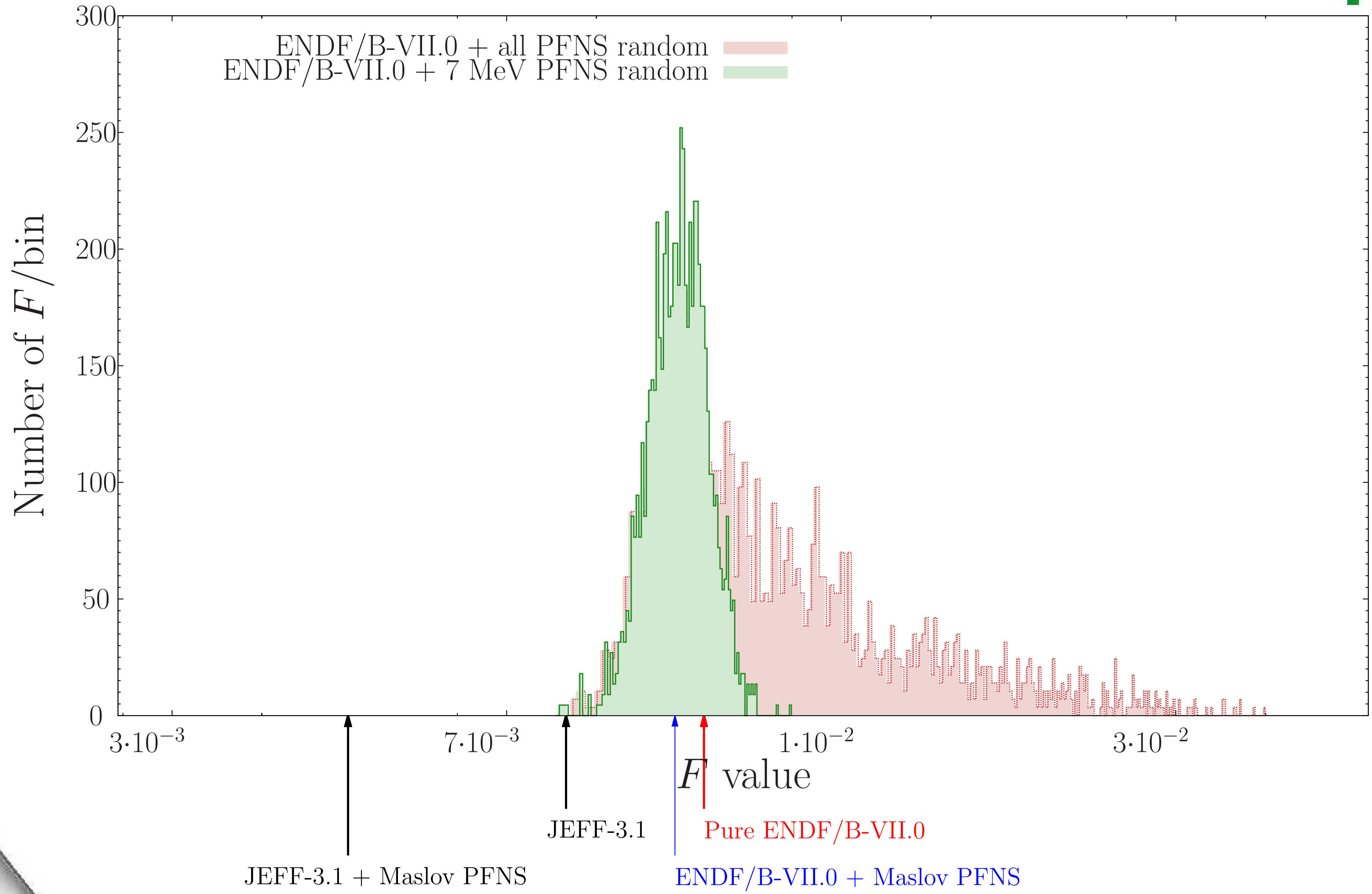
Example 2 on pfns of ^{239}Pu with only 7 fast benchmarks



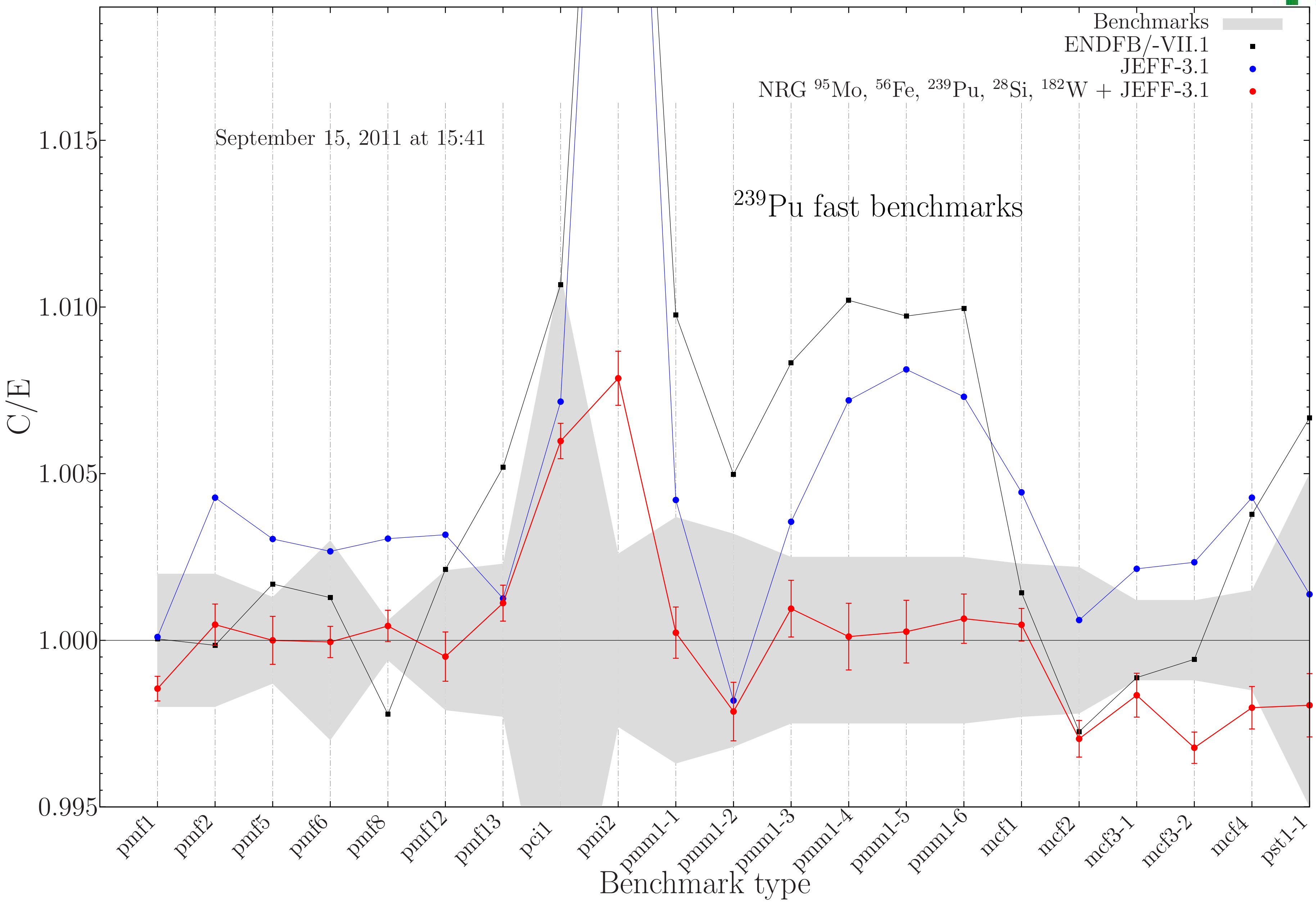
Example 2 on pfns of ^{239}Pu with only 7 fast benchmarks



Example 2 on pfns of ^{239}Pu with only 7 fast benchmarks



Petten method: *best* ^{239}Pu for the ANDES project



Petten method: second example on natural copper and Oktavian benchmark

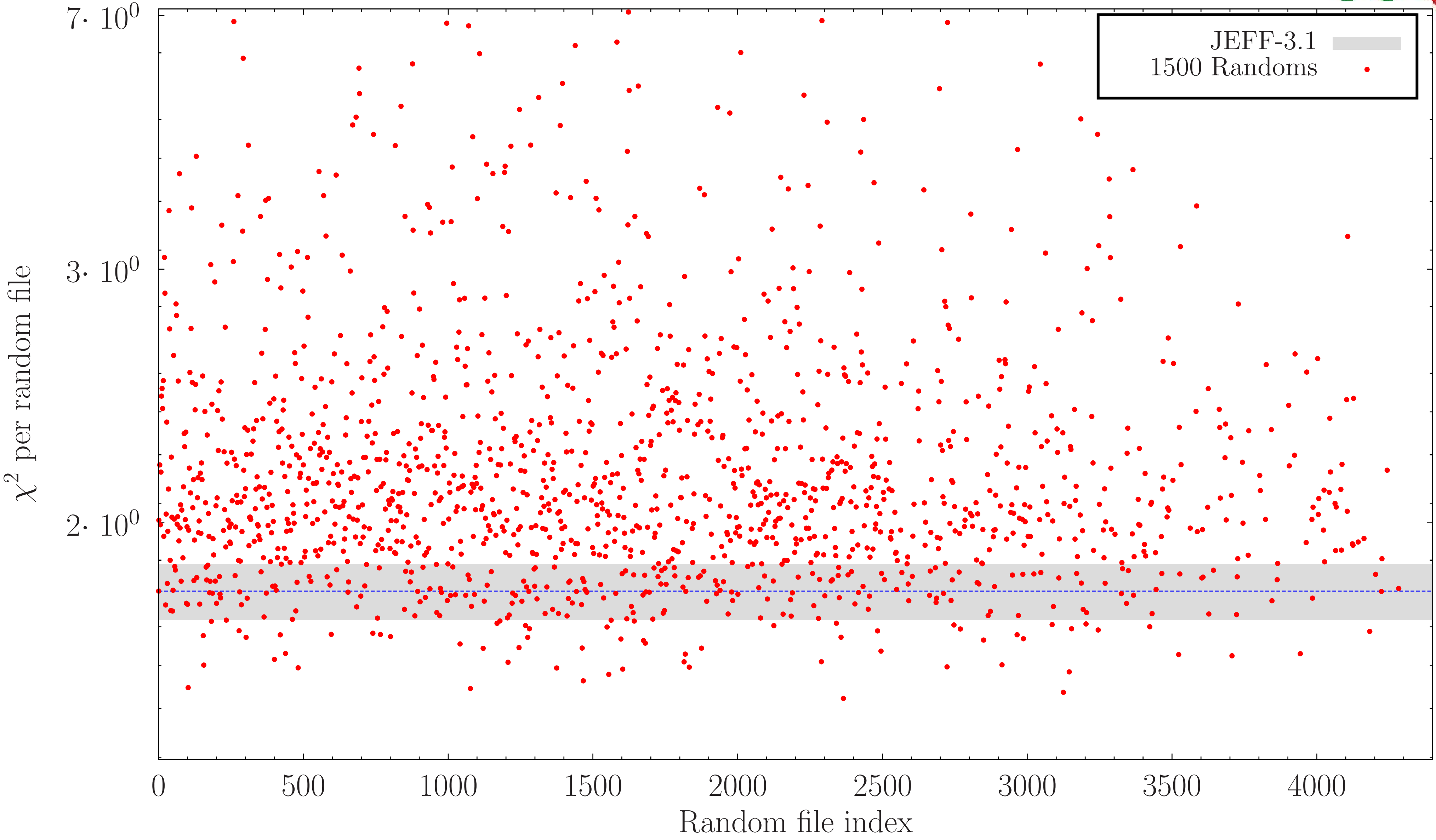
Name	weight	Name	weight	Name	weight	Name	weight
hmf22	1	hmf60	1	hmf67	2	hmf72	1
imf10	1	imf14	2	imf1	8	mmf11	4
pmf13	1	pmf5	1	hmi1	1	hmi6	4
hmt16	1	hmt6	9	hmt8	1	hst10	4
hst13	4	hst32	1	hst38	30	hst39	6
hst9	4	lct1	8	lct10	9	lct16	9
lct17	10	lct19	3	lct2	5	lct3	9
lct5	9	lct51	9	lct60	9	lmt1	1
lst18	6	pst3	8	Oktavian-n	135	Oktavian-γ	75

Criticality benchmark total weight: 392

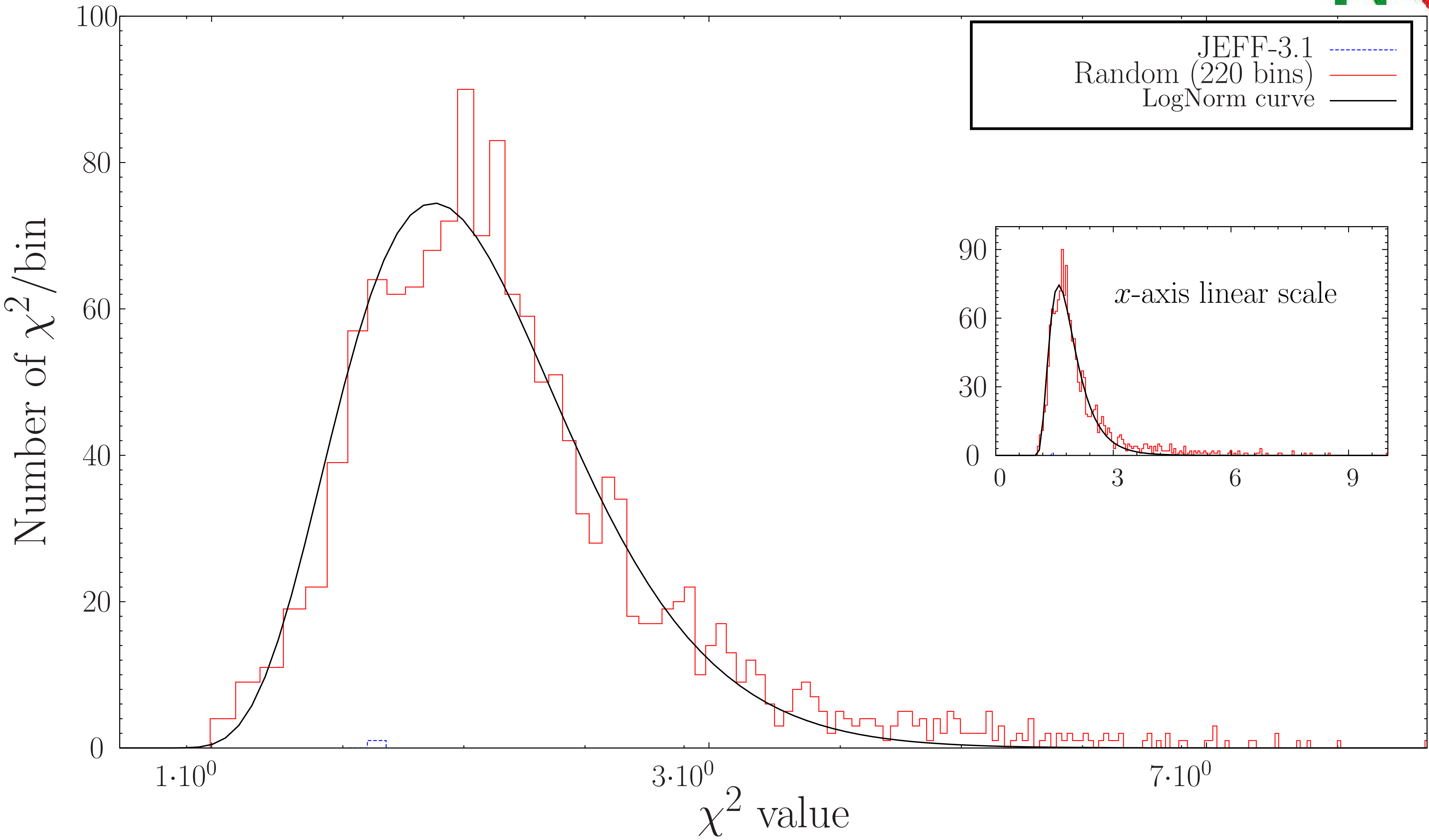
Reaction	Energy (MeV)	weight	Reaction	Energy (MeV)	weight
^{65}Cu(n,el)	8	4	^{63}Cu(n,el)	5	4
^{65}Cu(n,el)	10	4	^{63}Cu(n,el)	7	4
^{65}Cu(n,el)	11	4	^{63}Cu(n,el)	10	4
^{65}Cu(n,γ)	0.5	4	^{63}Cu(n,γ)	0.5	4
^{65}Cu(n,γ)	1.0	4	^{63}Cu(n,γ)	1.0	4
^{65}Cu(n,γ)	2.0	4	^{63}Cu(n,γ)	2.0	4
^{65}Cu(n,inl)	14.5	4	^{63}Cu(n,γ)	3.0	4
^{65}Cu(n,2n)	10.5	4	^{63}Cu(n,inl)	13.5	4
^{65}Cu(n,2n)	12	4	^{63}Cu(n,2n)	11.5	4
^{65}Cu(n,2n)	13	4	^{63}Cu(n,2n)	20	4
^{65}Cu(n,2n)	15	4			
^{65}Cu(n,2n)	17	4			

Experimental data total weight (EXFOR): 88

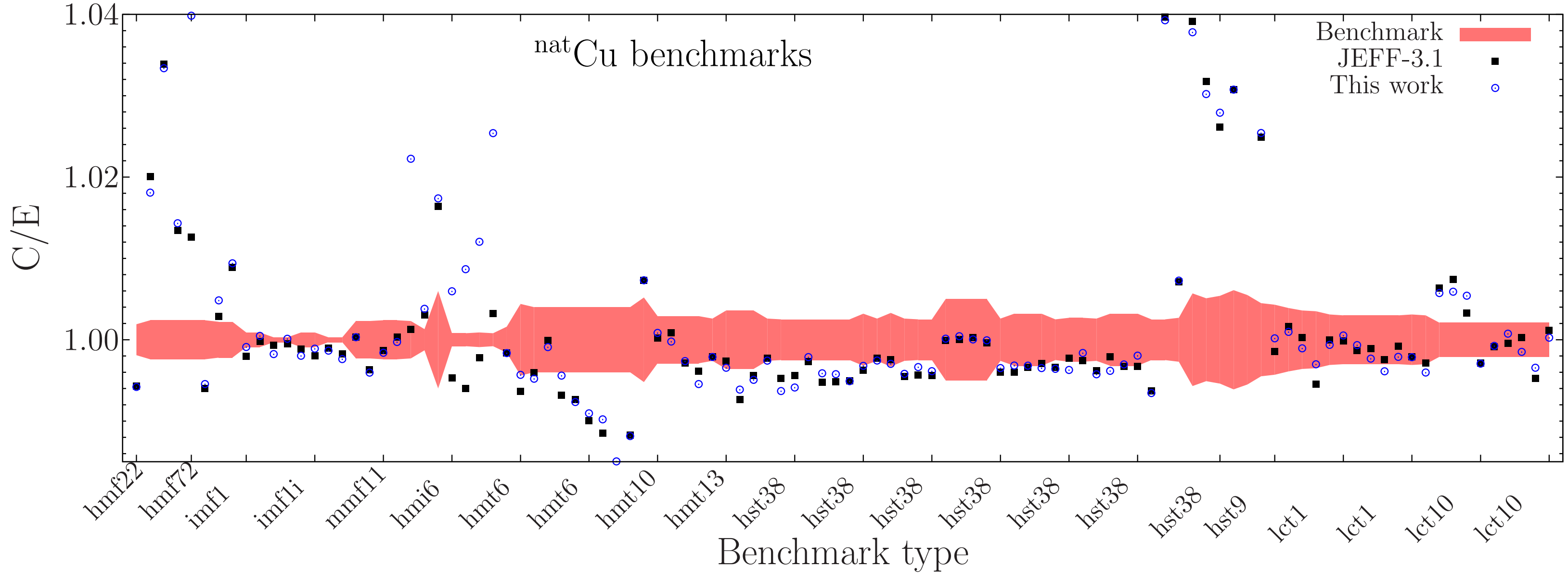
Petten method: second example on natural copper and Oktavian benchmark

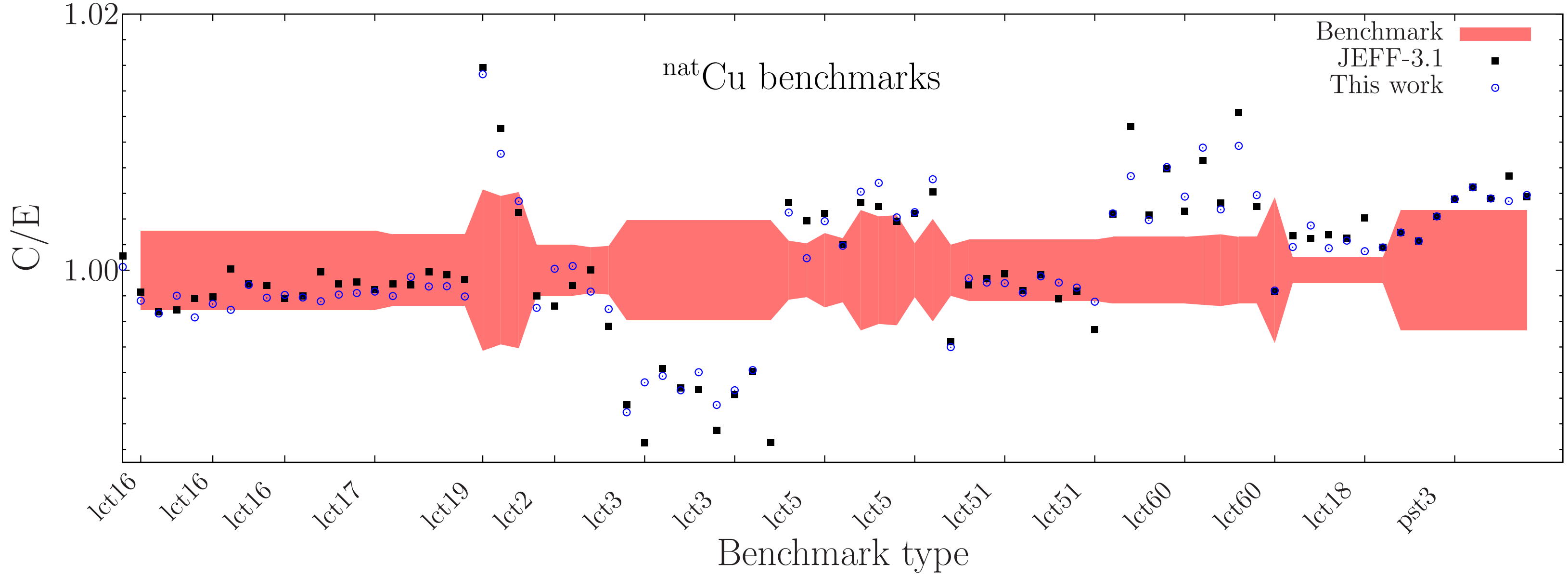


Petten method: second example on natural copper and Oktavian benchmark

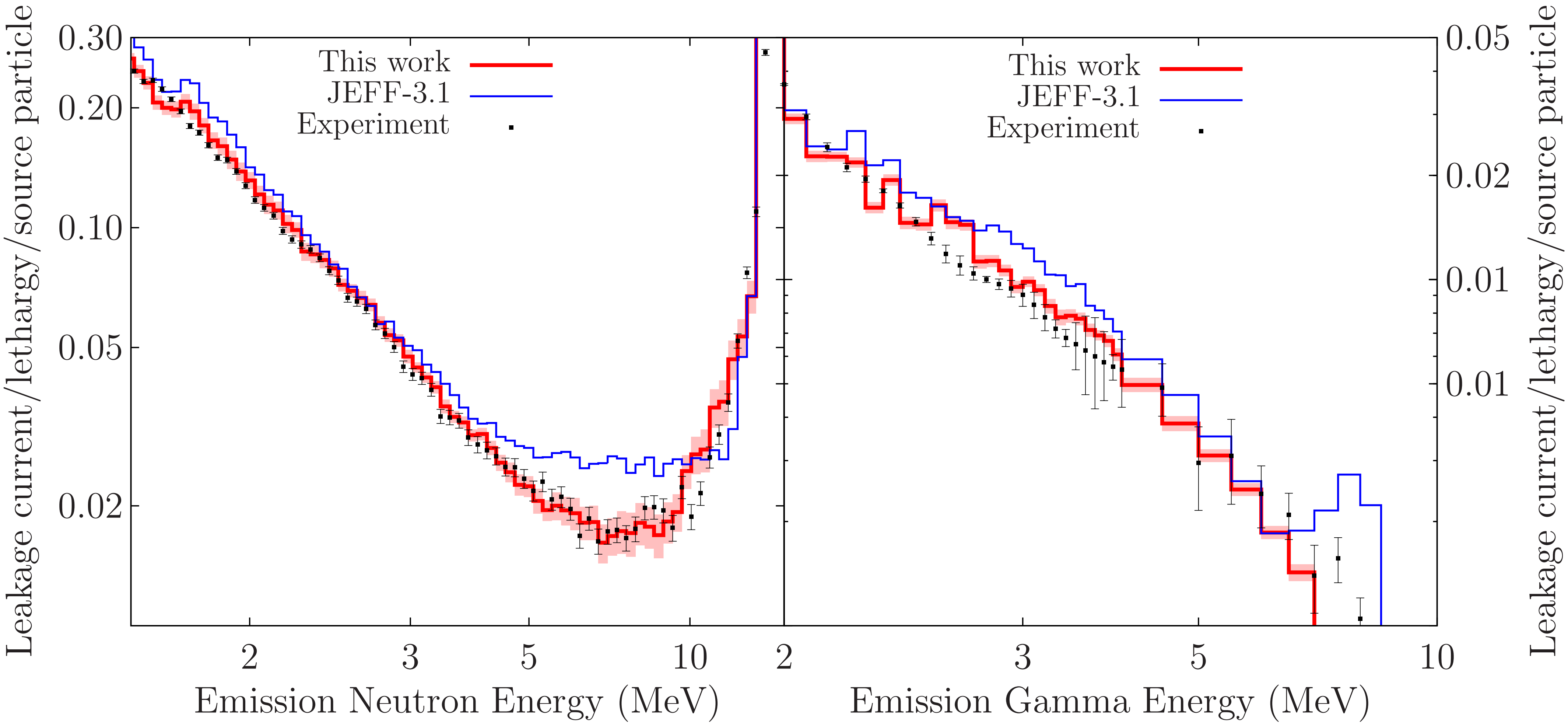


Petten method: second example on natural copper and Oktavian benchmark

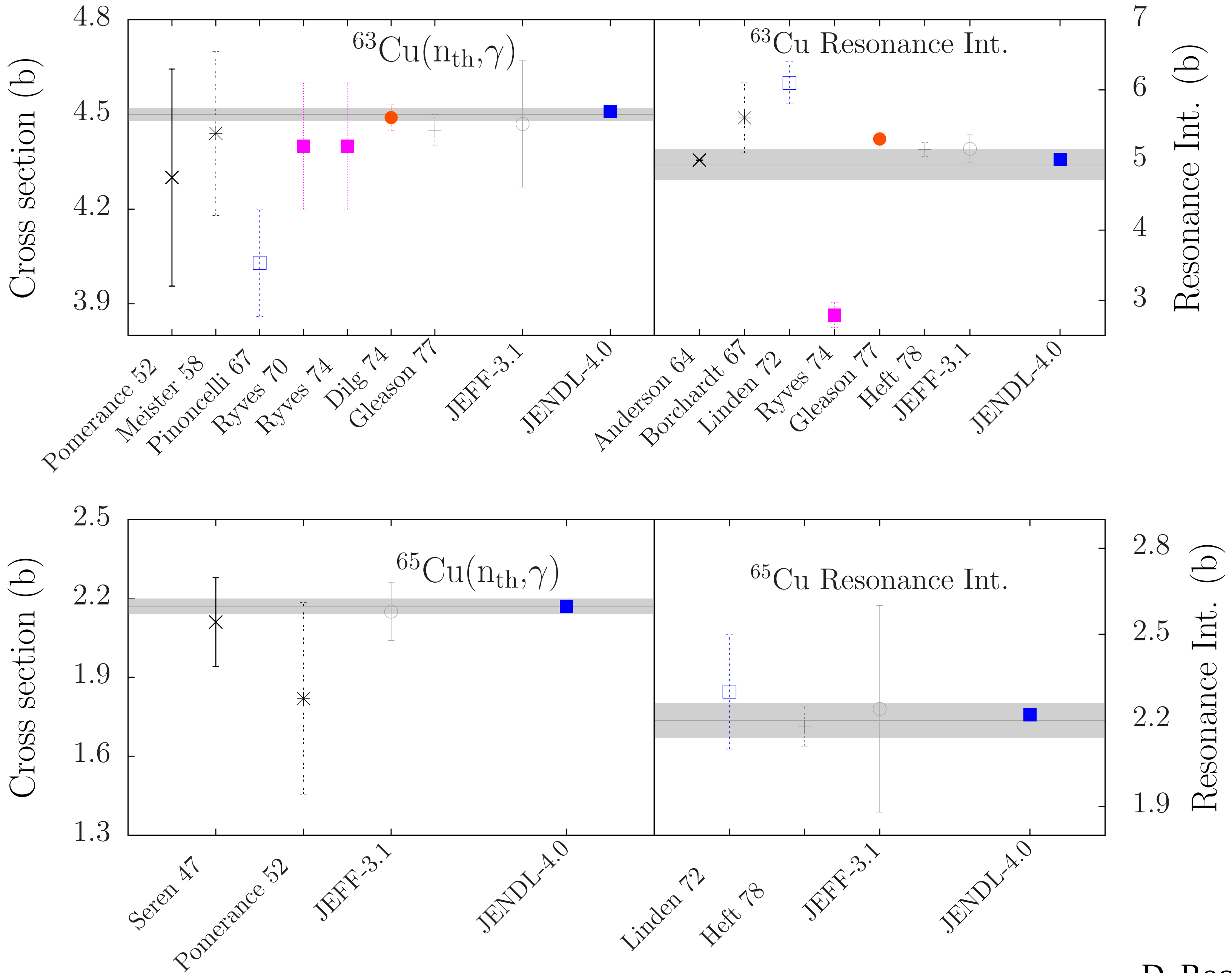




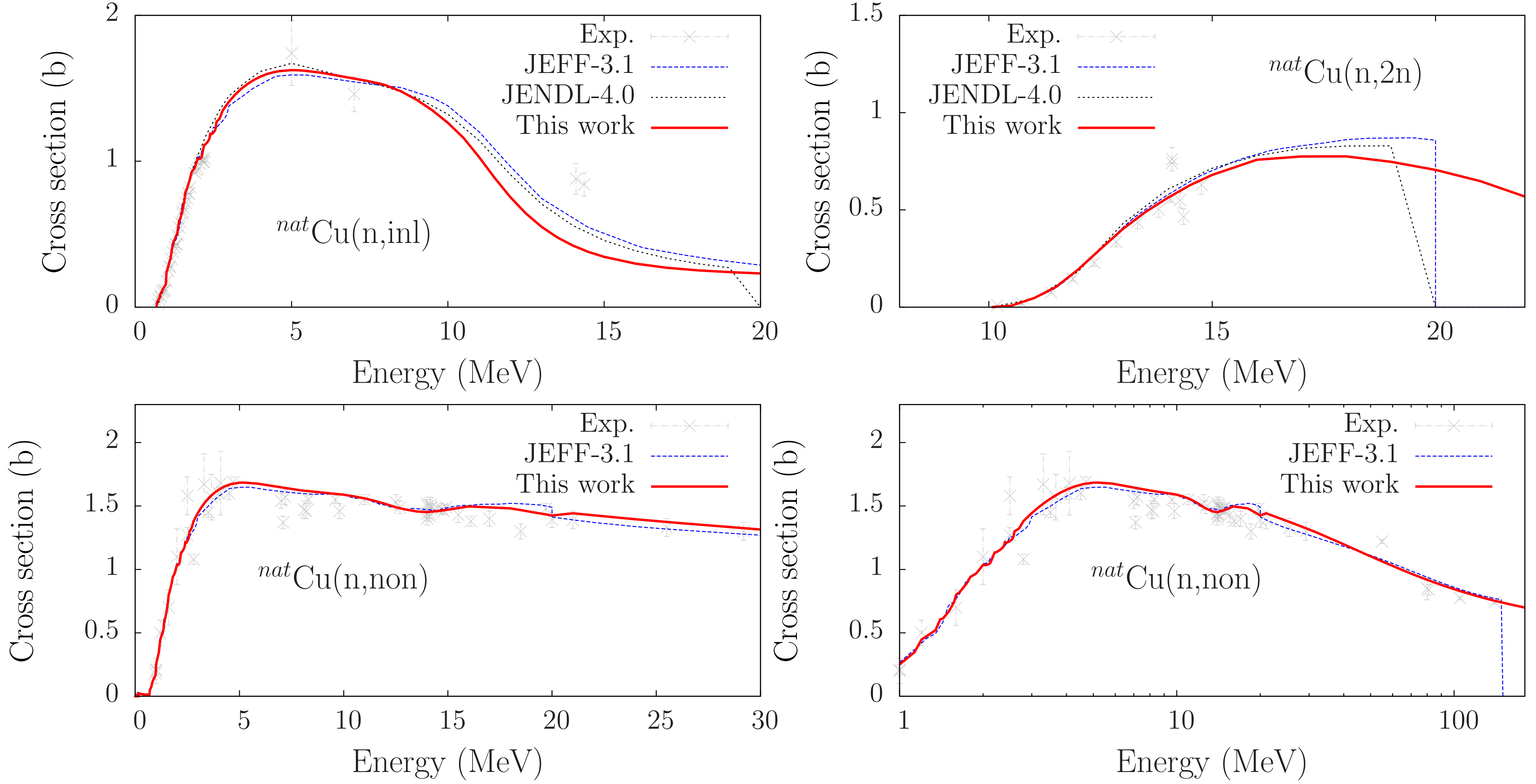
Petten method: second example on natural copper and Oktavian benchmark



Petten method: second example on natural copper and Oktavian benchmark



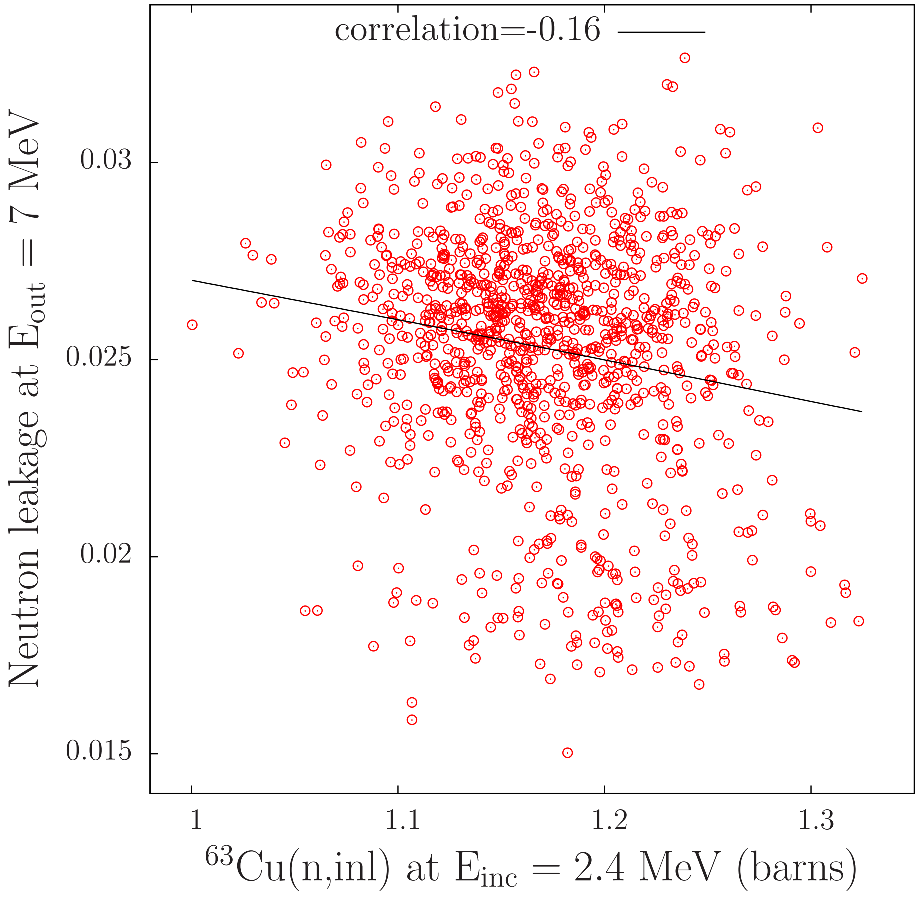
Petten method: second example on natural copper and Oktavian benchmark



Petten method: Correlation factors (instead of sensitivity)

$$\rho_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{(n-1)s_x s_y}$$

with x_i the random cross sections, $\bar{x}$ the average cross section, y_i the random k_{eff}, $\bar{y}$ the average k_{eff} and s_x and s_y their standard deviations.

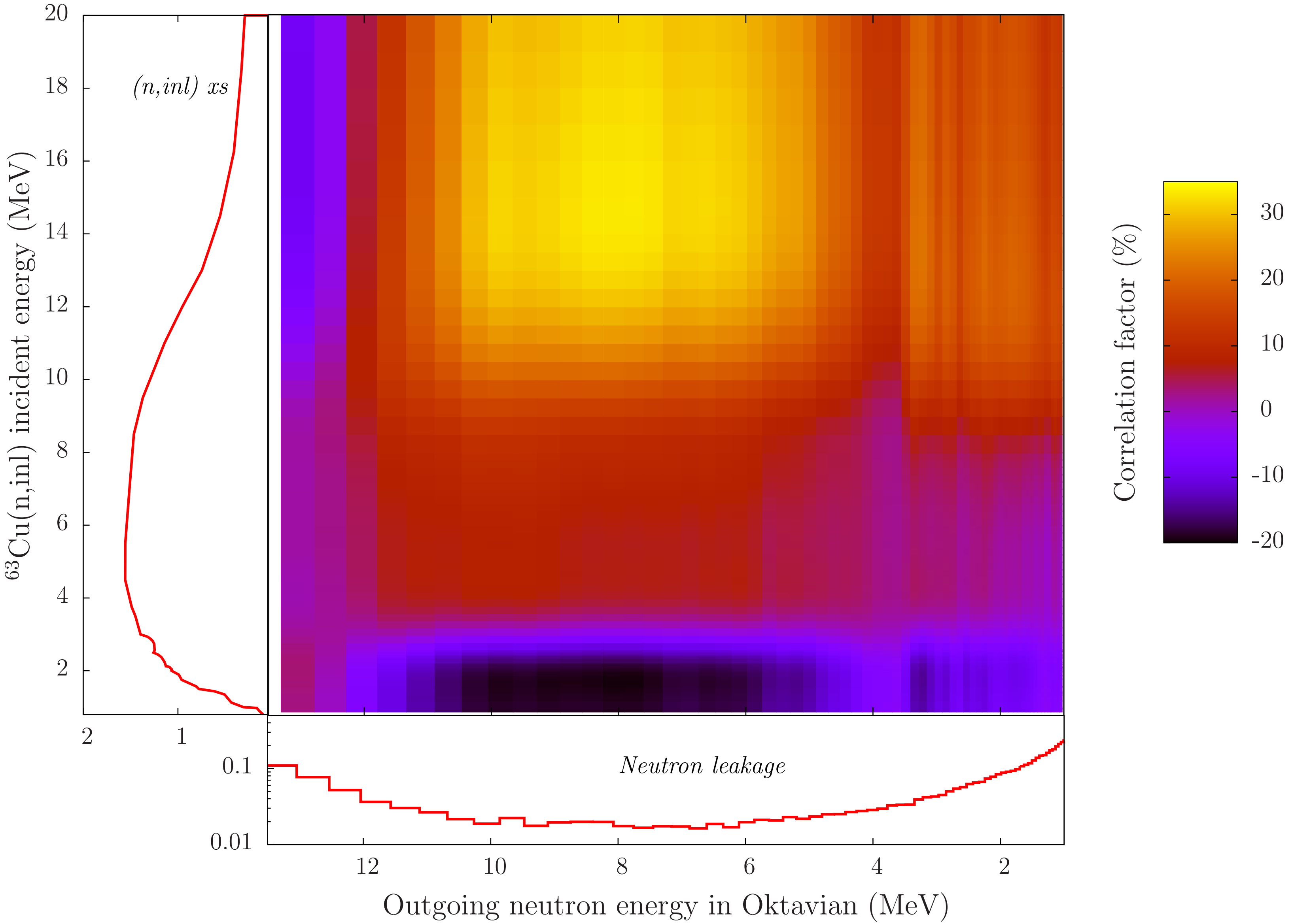


Petten method: Correlation factors (instead of sensitivity)

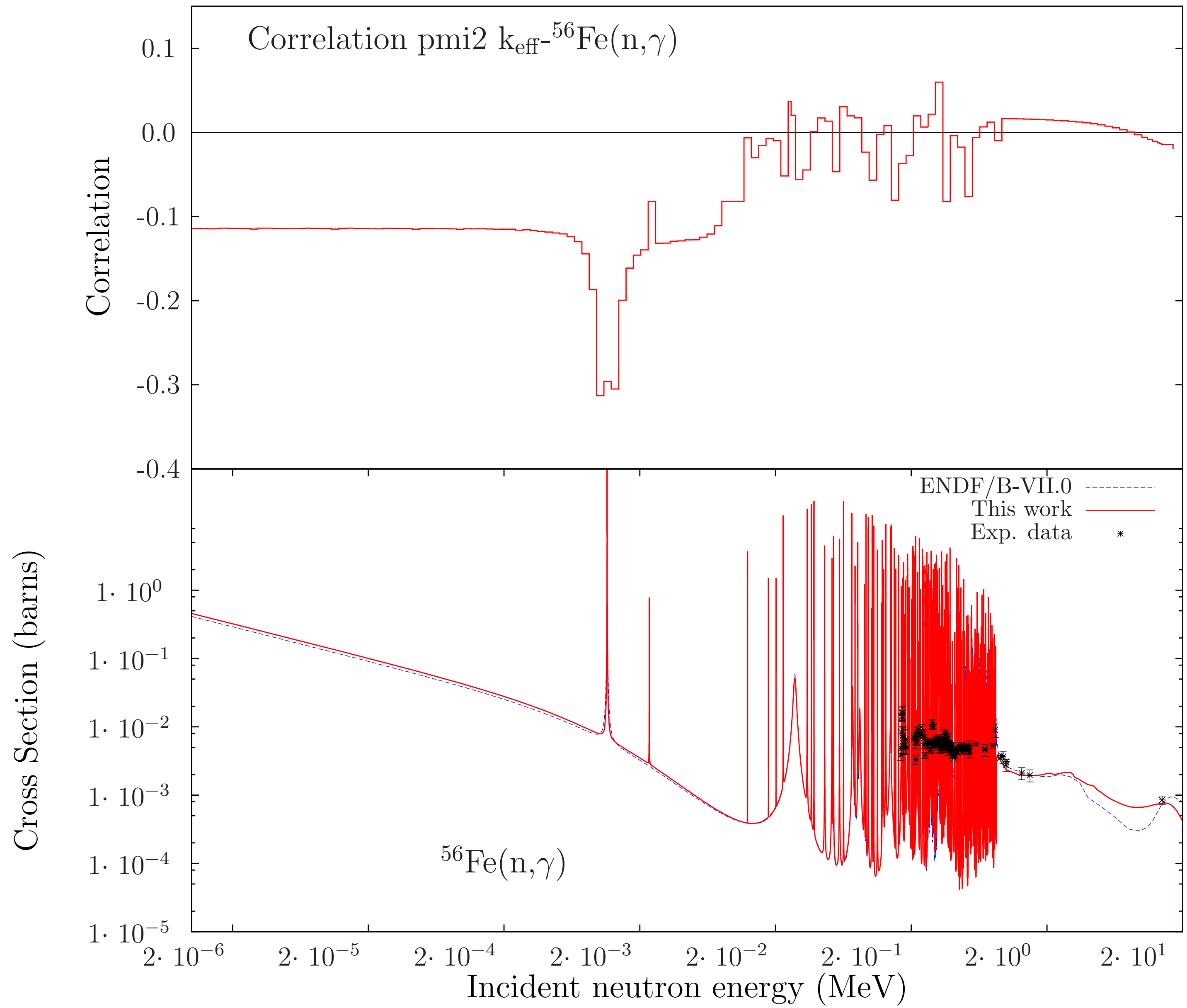
Table 2: Correlation factors between the Cu Oktavian neutron leakage benchmark and nuclear data (at given incident and outgoing energies).

E_{out} Oktavian	Reaction	E_{in} neutron	ρ_{xy}
7 MeV	^{63}Cu(n,inl)	2.4 MeV	-0.13
7 MeV	^{63}Cu(n,inl)	13 MeV	-0.35
7 MeV	^{63}Cu(n,2n)	20 MeV	-0.13
7 MeV	^{63}Cu(n,el)	7 MeV	0.17
7 MeV	^{65}Cu(n,inl)	14 MeV	0.01
7 MeV	^{65}Cu(n,2n)	11 MeV	0.01
7 MeV	^{65}Cu(n,el)	10 MeV	0.03
7 MeV	^{65}Cu(n,γ)	2 MeV	0.00

Petten method: second example on natural copper and Oktavian benchmark



Petten method: Correlation factors (proportional to sensitivity)



Petten method: third (and last) example on thermal scattering data H in H_2O

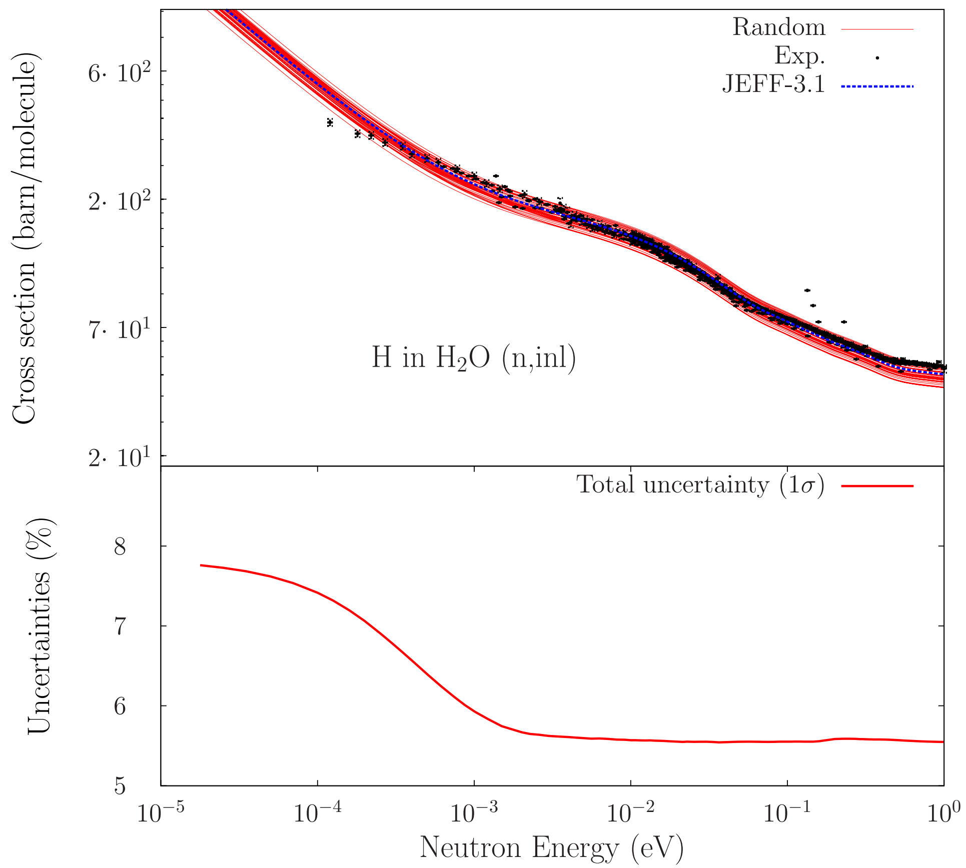
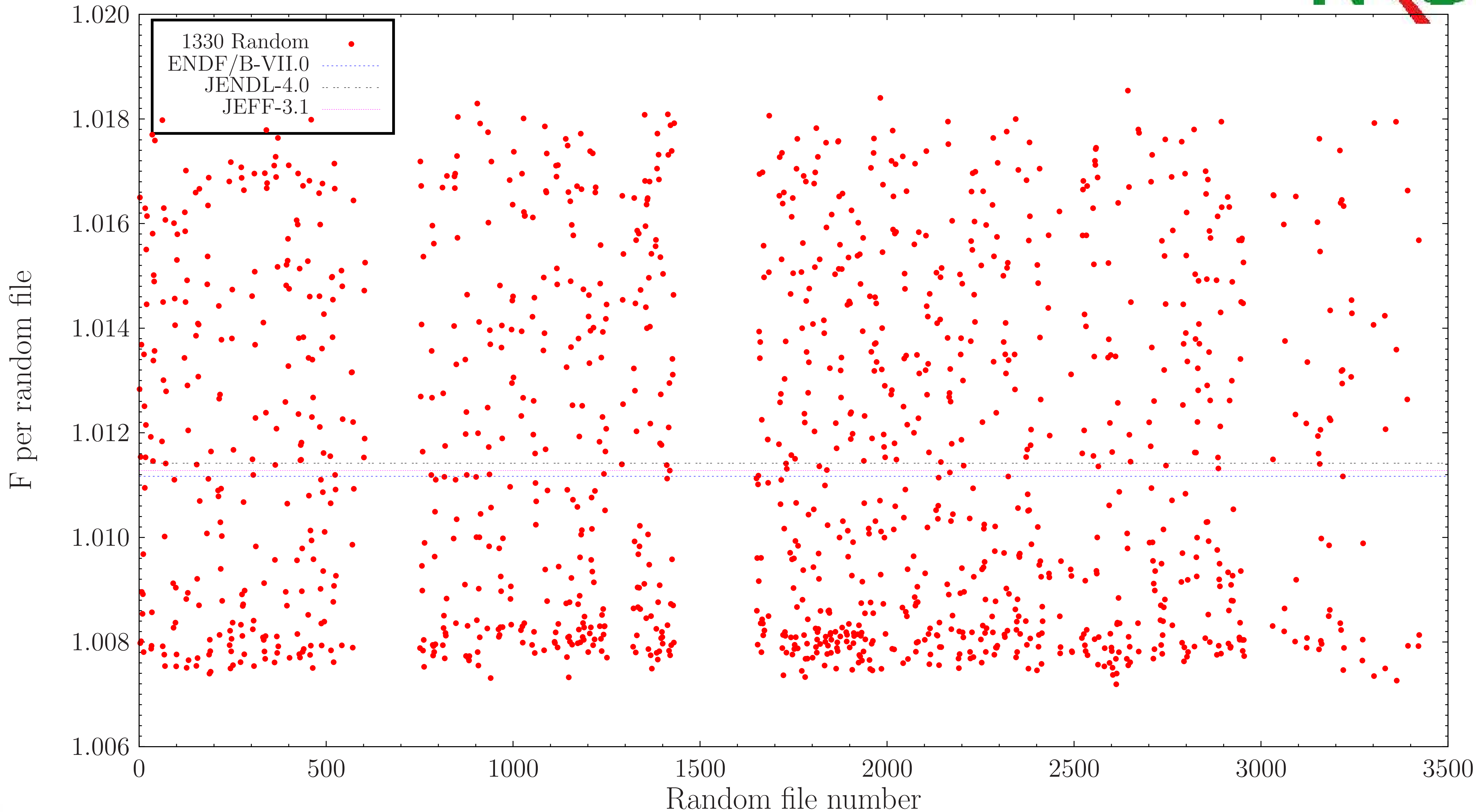


Table 3: List of thermal benchmarks selected for the random search.

Name	Cases	Name	Cases
pst12	22	pst1	6
lct7	10	lct6	18
lst4	7	lmt1	1
ict3	2	hst32	1
hst42	8		

$$F = 10^{\sqrt{\frac{1}{N}\sum(\log(E_i)-\log(C_i))^2}} \quad (3)$$

Petten method: Example on thermal scattering data H in H_2O



F distance values for random H in H_2O files (dots), compared to F for existing libraries (lines).

Petten method: Example on thermal scattering data H in H_2O