Neutron, Proton, Deuteron activation-transmutation files: n,p,d-FENDL-3/A

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EAF-2010

66256 neutron induced reactions

5096 important reactions

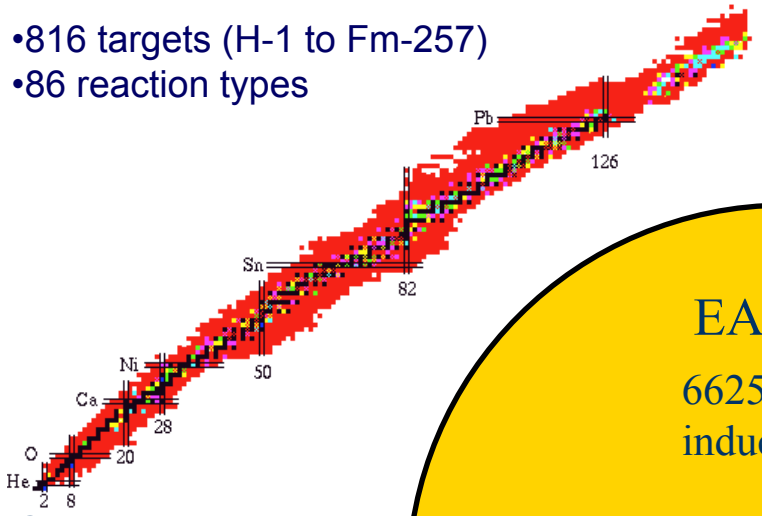
2265 major reactions

1728 reactions with any experimental data

470 reactions with integral data

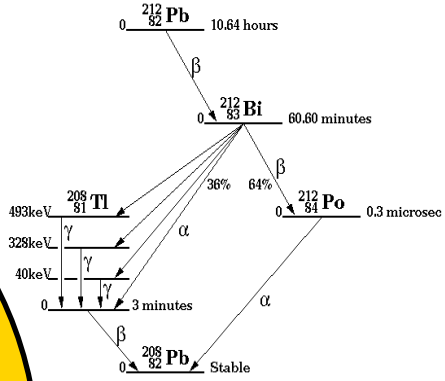
Cross sections

- 816 targets (H-1 to Fm-257)
- 86 reaction types



Decay data

- 2,233 nuclides
- Stables and isomeric states ($T_{1/2}$ > 1s)



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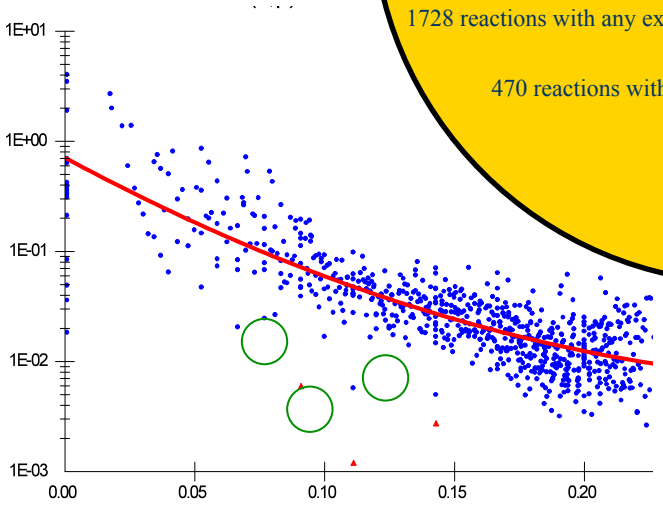
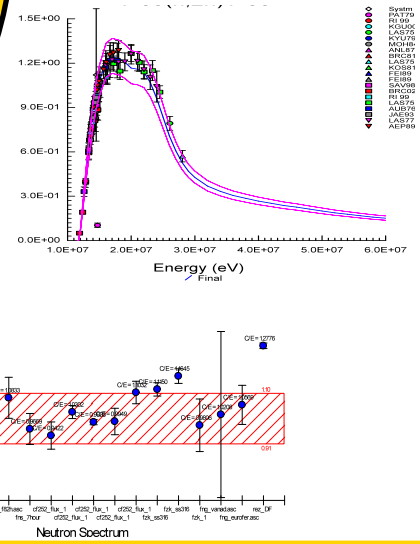


Validation: C/E



EAF-2010 = FENDL-3.0/A

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87 simple particles reactions = MT's

MT	Particles
2	n
4	n'
5	anything
11	2nd
16	2n
17	3n
18	fission
22	nα
23	n3α
24	2nα
25	3nα
28	np
29	n2α
30	2n2α
32	nd
33	nt
34	n^{3}He
35	nd2α
36	nt2α
37	4n
41	2np
42	3np
44	n2p

MT	Particles
45	npα
102	g
103	p
104	d
105	t
106	^{3}He
107	α
108	2α
109	3α
111	2p
112	pα
113	t2α
114	d2α
115	pd
116	pt
117	dα
152	5n
153	6n
154	2nt
155	tα
156	4np
157	3nd
158	n'dα

MT	Particles
159	2npα
160	7n
161	8n
162	5np
163	6np
164	7np
165	4nα
166	5nα
167	6nα
168	7nα
169	4nd
170	5nd
171	6nd
172	3nt
173	4nt
174	5nt
175	6nt
176	2nh
177	3nh
178	4nh
179	3n2p
180	3n2α
181	3npα

MT	Particles
182	dt
183	n'pd
184	n'pt
185	n'dt
186	n'ph
187	n'dh
188	n'th
189	n'tα
190	2n2p
191	ph
192	dh
193	hα
194	4n2p
195	4n2α
196	4npα
197	3p
198	n'3p
199	3n2pα
200	5n2p

Only 6 of the new channels do not output a neutron

Actual MT black (39)

New MT green (48)

Approved during the Nov. 2010 CSWEG meeting

ENDF-6 Format Manual - xxx 2011 Revision

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MT Values

- Grid of reactions including all (old) **37 MT numbers** previously defined and some recently added, **+ 49 MT**

	N-7	N-6	N-5	N-4	N-3	N-2	N-1	N	N+1
Z	(n,8n) 161	(n,7n) 160	(n,6n) 153	(n,5n) 152	(n,4n) 37	(n,3n) 17	(n,2n) 16	(n,n') 4	(n,γ) 102
Z-1					(n,2nt) 154	(n,nt), (n,2np) 33,42	(n,t), (n,nd) 105,32,41	(n,d), (n,np) 104, 28	(n,p) 103
Z-2	(n,6na) 167		(n,4na) 165	(n,3na) 25, **200**	(n,2na) 24	(n,n'a) 22	(n,a), (n,nh) 107,34,116	(n,h), (n,pd) 106,44,115	(n,2p) 111
Z-3					(n,2npa) 159	(n,da),(n,npa) 117,45	(n,pa) 112		(n,3p) 197
Z-4			(n,2n2a) 30	(n,n2a) 29	(n,2a) 108				
Z-5		(n,nt2a) 36	(n,t2a) 113,35	(n,d2a) 114					
Z-6		(n,n3a) 23	(n,3a) 109						

Classical MT's
New MT's

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EAF2ENDF processes

- Transforms EAF-format into ENDF-6 format
- Modified to handle branching ratio
- Modified to handle the recently defined MT's
- Groups partial channels in a complete data file for each of the 816 target isotopes
- Main transformation: MF3 (EAF) --> MF3/8/9/10 (ENDF-6)
  - add MF-1 and MF-2
- All cross sections up to 60 MeV
- Automatically starts CHECKR, FIZCON, and PSYCHE
- Allow the use of all ENDF utility code, PREPRO-2011 and NJOY-99.364
- The IAEA (V. Zerkin) merged EAF-2010 in ENDF-6 format and EAF-2010_UN → MF33/40

Final release, bug correction; mid November

EAF-2010 into ENDF-6 = n-FENDL-3.0/A

- MF-1 General information, comments
  - » Including the original EAF comments lines
- MF-2 Resonance parameters
  - » skeleton ; r = 1.35x($A^{1/3}$)
  - » all resonant channels in PENDF (293.6 K)
- MF-3 Total cross section channels
- MF-8 Flag, file pointer, dictionary (for NJOY only)
  - » either to MF-3/9 or MF-10
- MF-9 Isomeric branching ratio
  - » energy dependant
- MF-10 Split threshold reaction channels
- MF-33 Cross section covariance
- MF-40 Radionuclide production covariance

MF-3 and MF-10 cannot be populated simultaneously, total reaction channels are not stored when partials exist

Unified ENDF-6 file frame

MF	Description
1	General information, comments
2	Resonance parameter, scattering radius
3	Total reaction channels
6	Radionuclide yields for MT-5
8	Flag, file pointer, dictionary
9	Isomeric branching ratio, for non threshold reaction
10	Split threshold reaction channels
33	Covariance of neutron cross sections
39	Covariance for radionuclides production yields
40	Covariance for production of radioactive nuclei

Toward a unified ENDF-6 formatted file frame
A. J. Koning ,D. Rochman ,J-Ch C. Sublet
CCFE-R(11) 16 (November 2011)

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Processing sequences

① Format checks: **moder, dictin, fixup, calendf, crectj6**
② MF-2 parameters: **recent, linear, reconr, calendf**
③ Doppler: **sigma1, broadr, calendf**
④ Heating, damage: **heatr**
⑤ RR & URR: **calendf, groupie, purr**
⑥ Gas production: **gaspr**
⑦ Activation: **activate, groupr, sixpak**
⑧ Multigroup : **groupie, groupr**
⑨ Graph checks: **evalplot, plotr, viewr, complot and ZVView**

All this is done respecting the ENDF-6 format

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Evaluated and Processed files

- The end results are fully compliant ENDF-6 formatted evaluated and processed files.
- All processing steps, sequences can be easily re-launched to account for any changes, modification, updates.
- Many intermediary steps, output listing or pre-processed files, add to the robustness of such system.

➢ The basic nuclear data and the processing steps are transferred to technology in a consistent and QA manner.

LLNL Generalized Nuclear Data format

- Lawrence Livermore National Laboratory (LLNL) is releasing the third version of a new "Generalized Nuclear Data" (or **GND**) format, designed to replace the ENDF-6 and LLNL's ENDL formats.
- The FUDGE package, a set of routines (written in Python) convert an existing ENDF-6 formatted file into this new XML format.
- By default, this package outputs the new format in XML, however for converting to HDF5, the XML2HDF5 tool can be used.

n-FENDL-3.0/A in GND format

- The fully ENDF-6 compliant pointwise forms of EAF-2010 have been converted in GND format ……and back in ENDF-6 format

  Zr90.endf6.orig

  Zr90.endf6.xml (rather human readable format)

  Zr90.endf6-covar.xml

  Zr90.endf6 ⬇ back to ENDF-6 !!

  Zr90.endf6.orig.noLineNumbers.cleanAndFixed

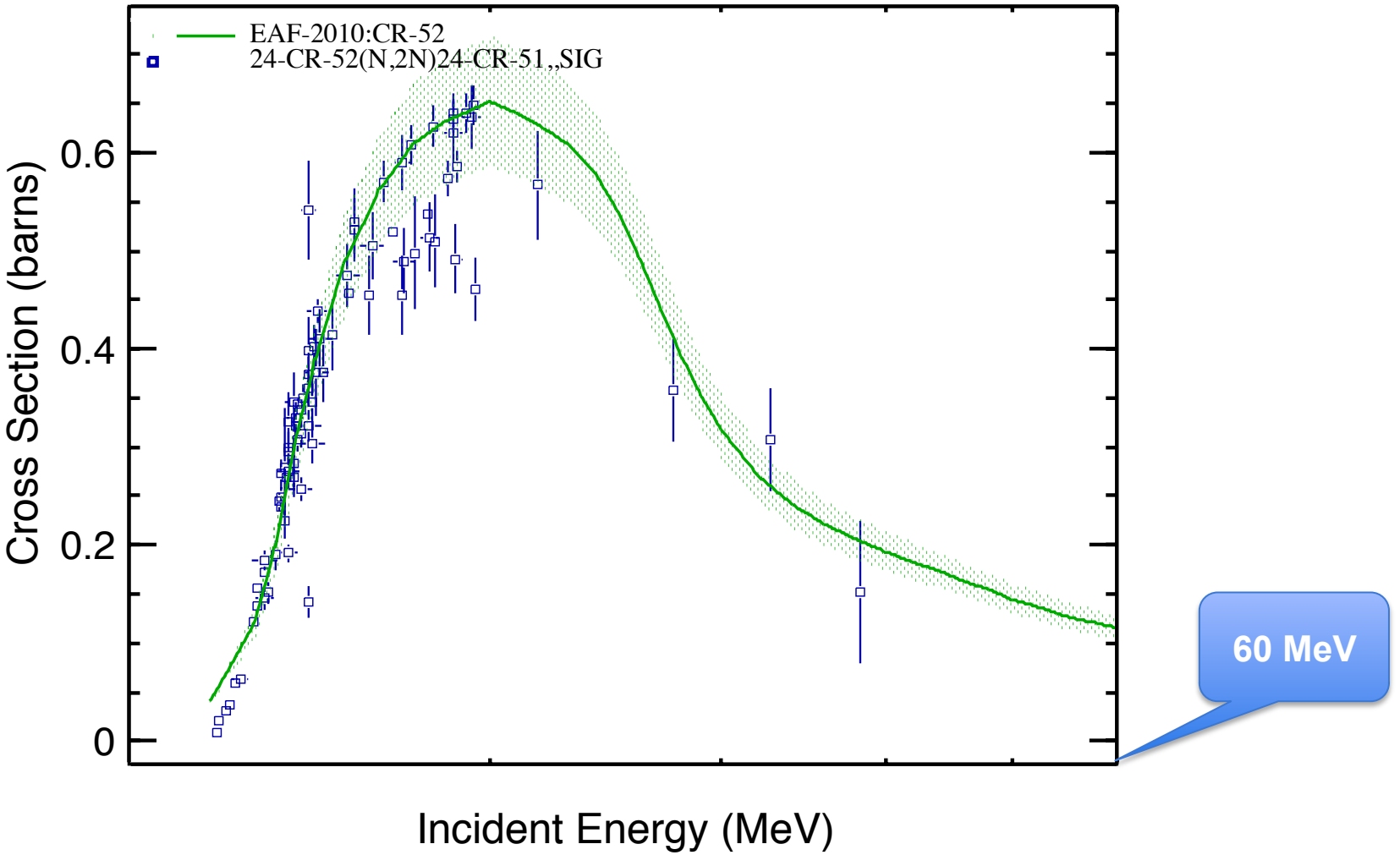
  Zr90.endf6.orig.noLineNumbers.clean

n-FENDL-3.0/A in GND format

- FUDGE-V.2 to FUDGE-V.3 to tackle EAF-2010
- This conversion tool pick-up ‘inconsistency” the utility codes did not !! - excitation levels
- GND is more robust than ENDF, less permissive, the physics contents can and has been be tighten up during the conversion (and back !!)
- Many utilitarian, plotting tools ‘plug-in’ easily into such a format
- This format has a place and a future in Nuclear Data world

Thanks to Caleb Mattoon at LLNL

IAEA Web site



EAF-2010 in ENDF-6 format with PREPRO, ZVview, EXFOR

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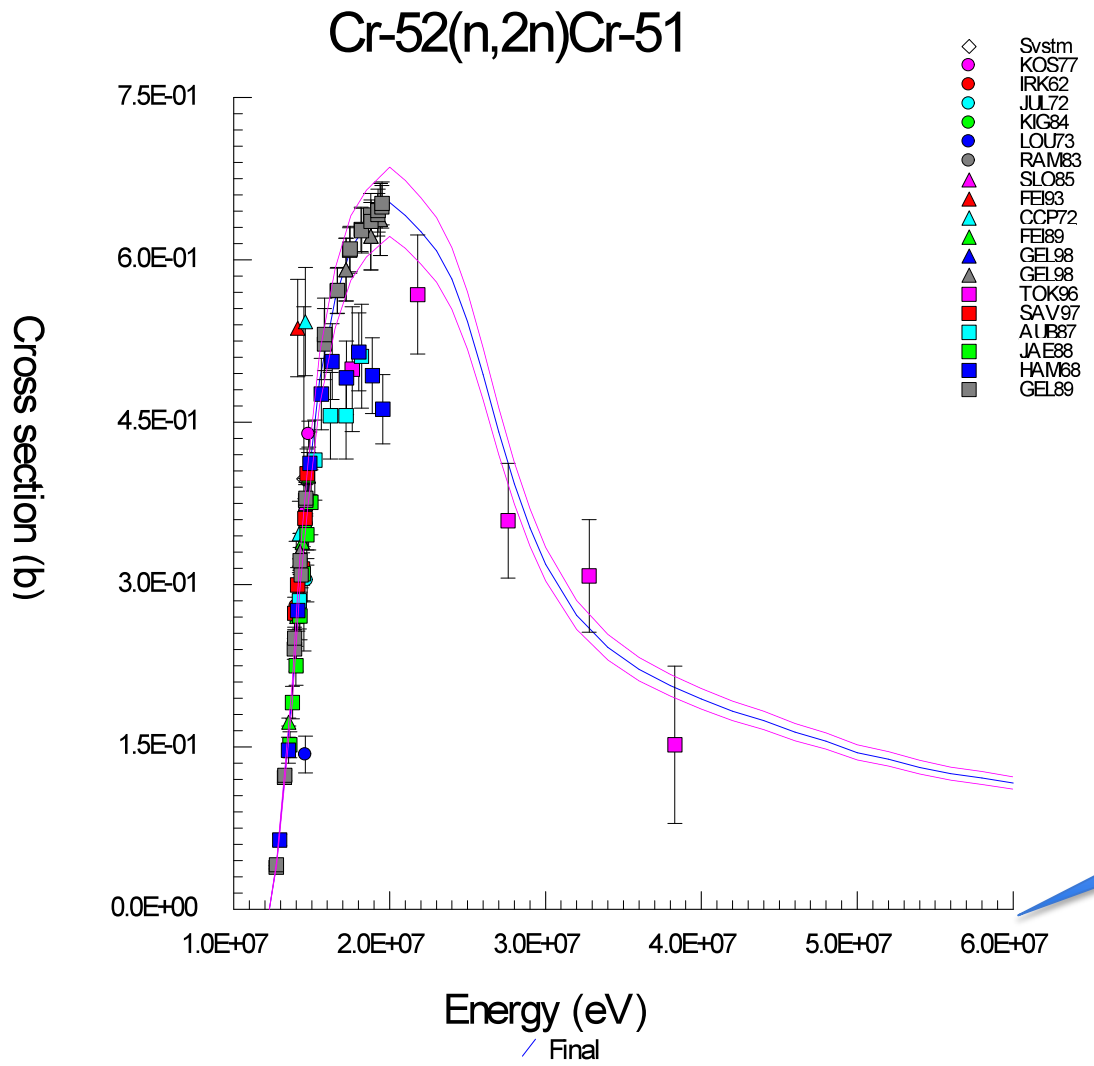
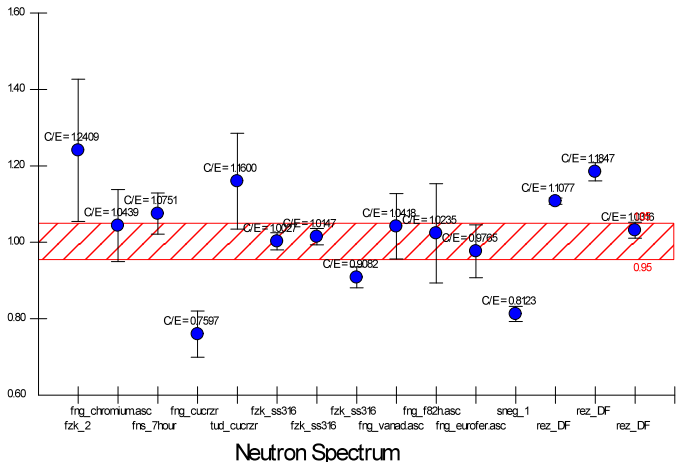
SAFEPAQ-II at CCFE





60 MeV

SAFEPAQ-II integral Validation

EAF-2010 in EAF format with SAFEPAQ-II

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Variance and uncertainty

Data	Standard deviation	Variance
A	Δ	Δ^2
50	0.05	0.0025

- The uncertainty correspond to the error factor

$$f = 1 + U$$

- The best estimate of the cross section uncertainty is

$$\sigma/f < \sigma < \sigma f$$

- Assuming that the uncertainty is 3 time the standard deviation

$$U = 3\Delta \ (U^2 \text{ in EAF\_UN})$$

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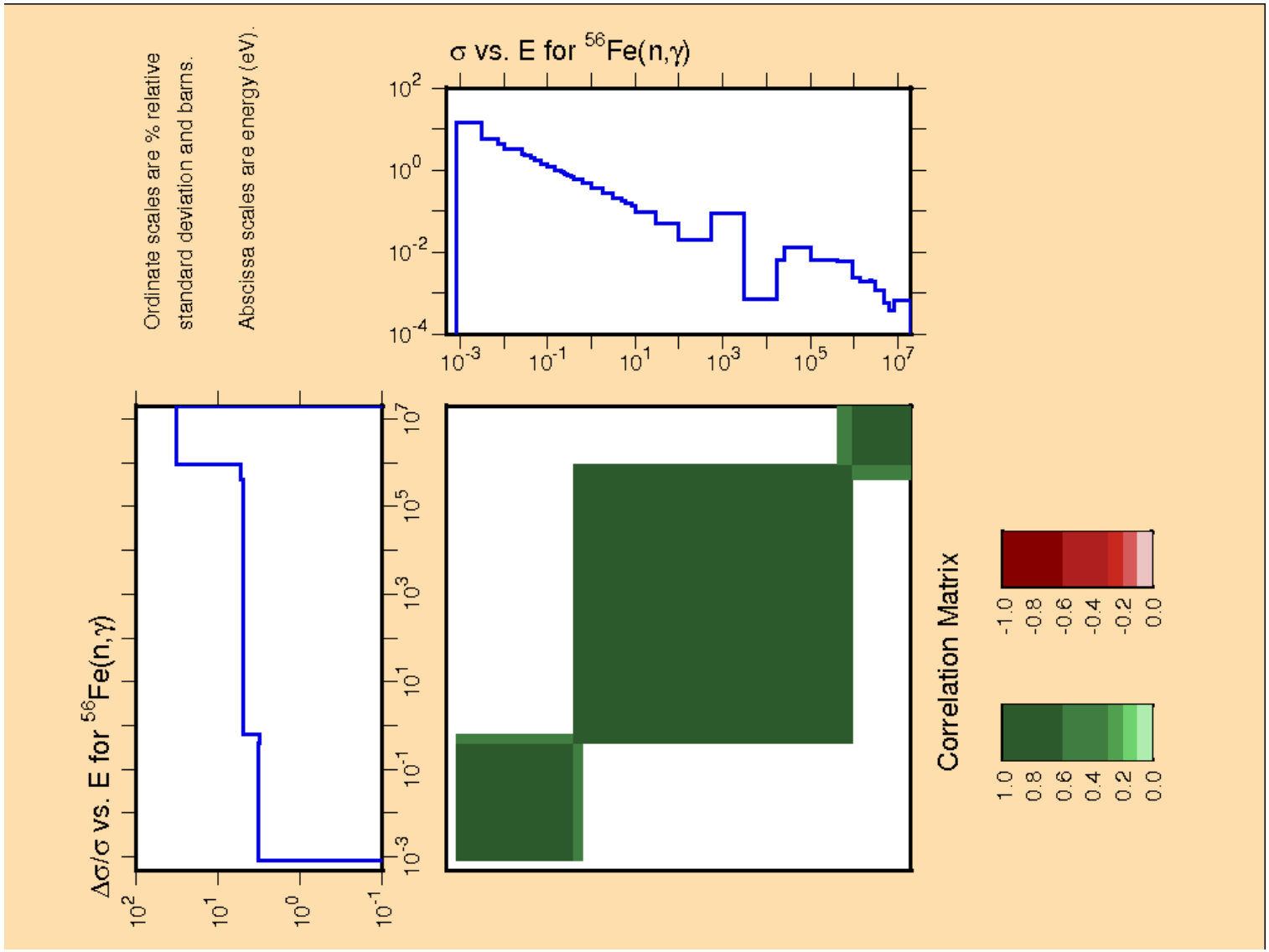
EAF uncertainty file

- Since 1994, EAF's library have been flanked by an uncertainty file, in pseudo MF-33 format.
- Prototype ENDF-6 formatted version of EAF has existed since EAF-2003, 2 to 4 groups MF-33.
- Fully compliant ENDF-6 format EAF-2010 version now includes MF-33 (cross sections) and MF-40 (radionuclide) covariance file, 60 MeV upper energy, 816 targets, 66256 channels.

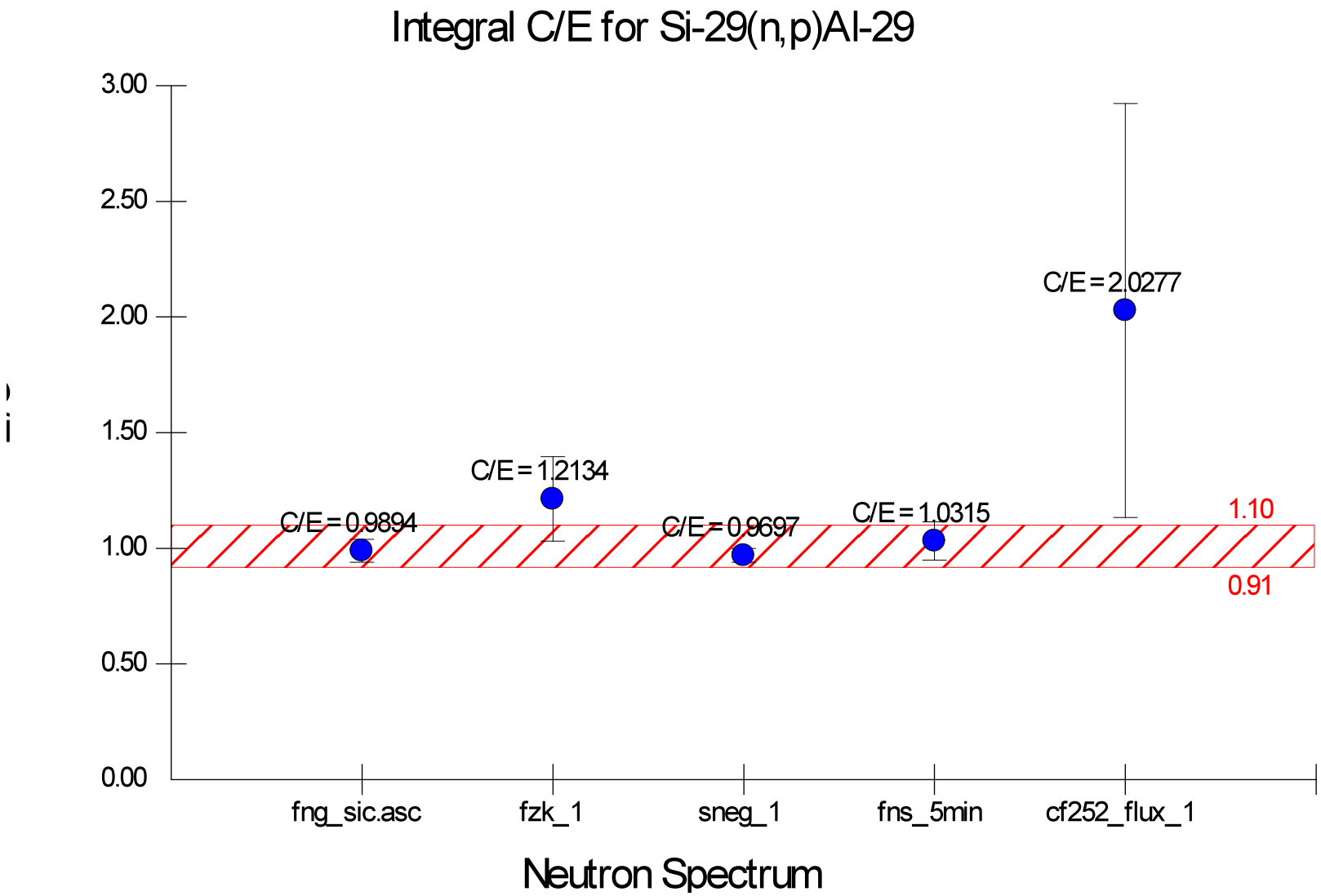
Format changes approved during the November 2010 CSWEG meeting, in the ENDF-6 Format Manual - dec 2011 Revision !!

EAF-2010 NJOY-ERRORR



60 MeV

Validated reactions - $^{29}Si(n,p)^{29}Al$



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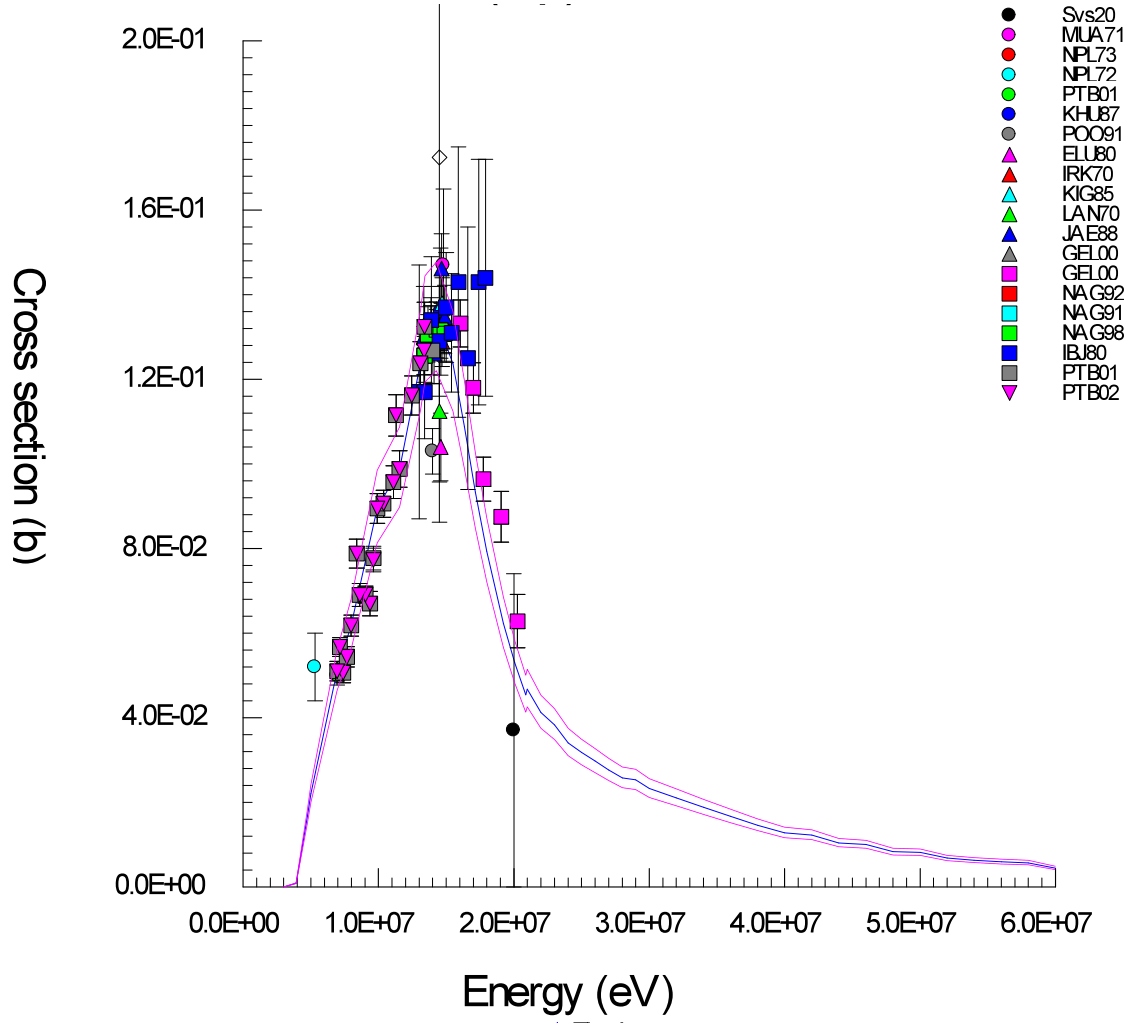
Validated reactions - $^{29}Si(n,p)^{29}Al$



Validated QS=6

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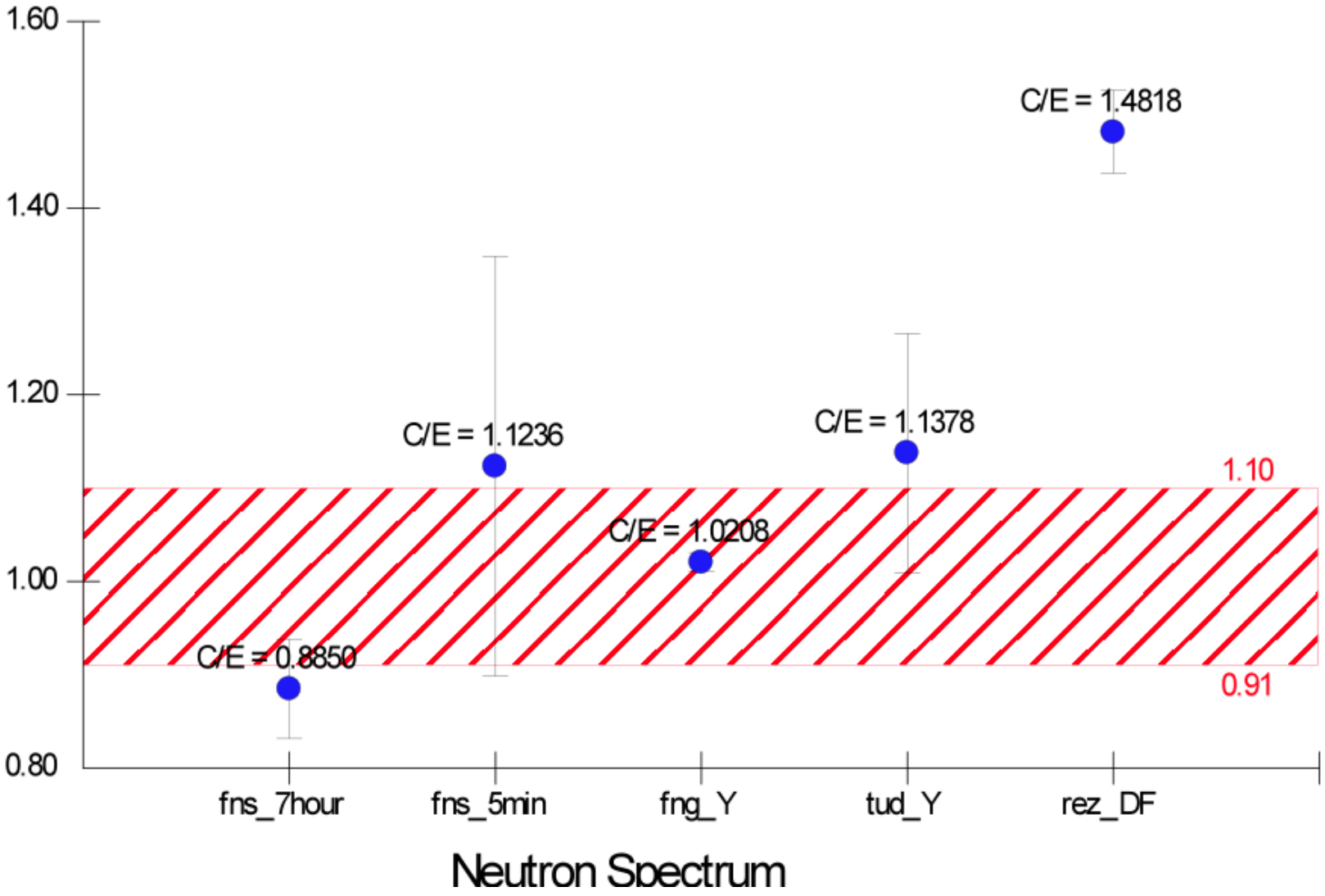
Validated reactions – $^{89}Y(n,2n)^{88}Y$



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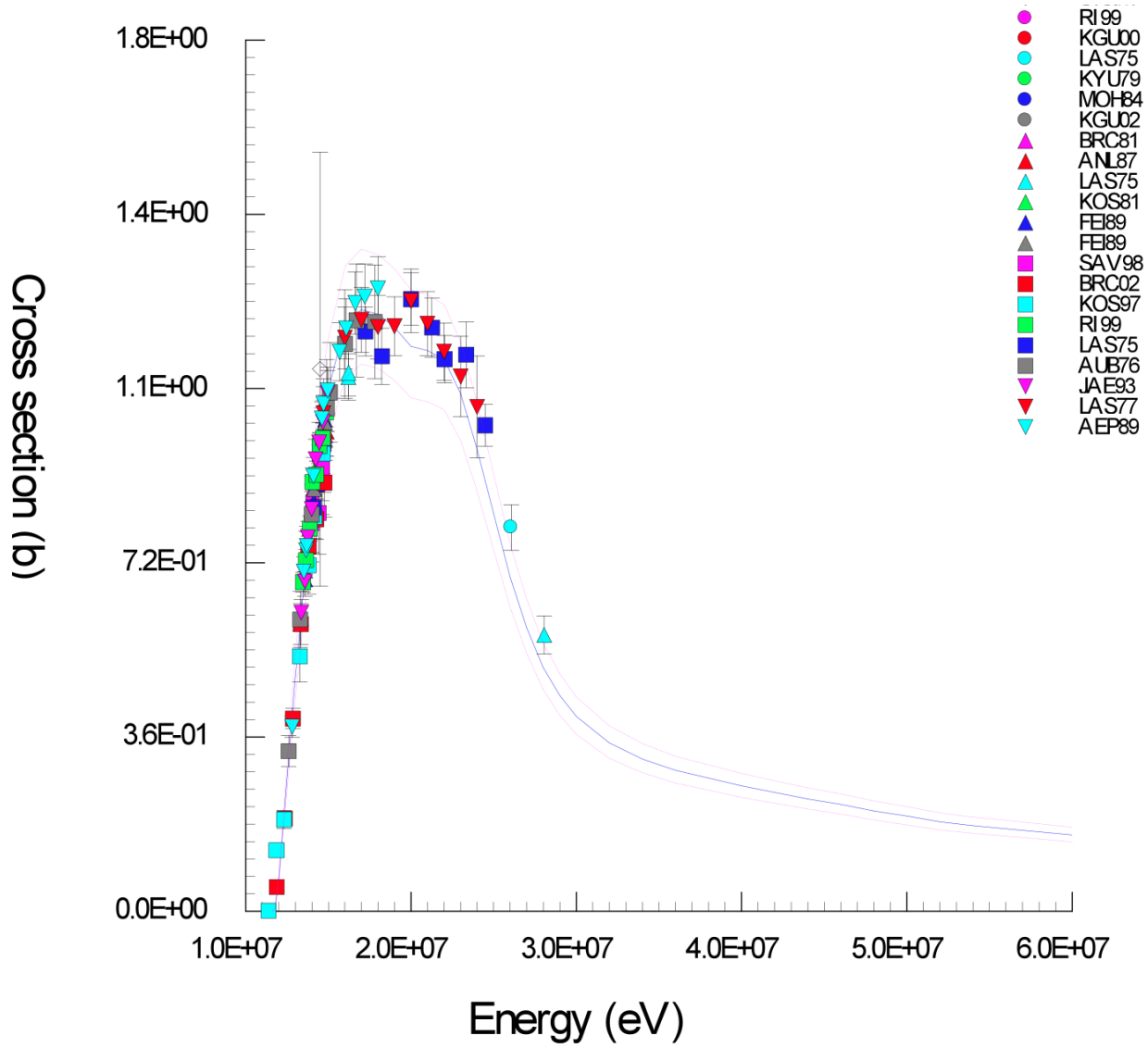
Validated reactions – $^{89}Y(n,2n)^{88}Y$



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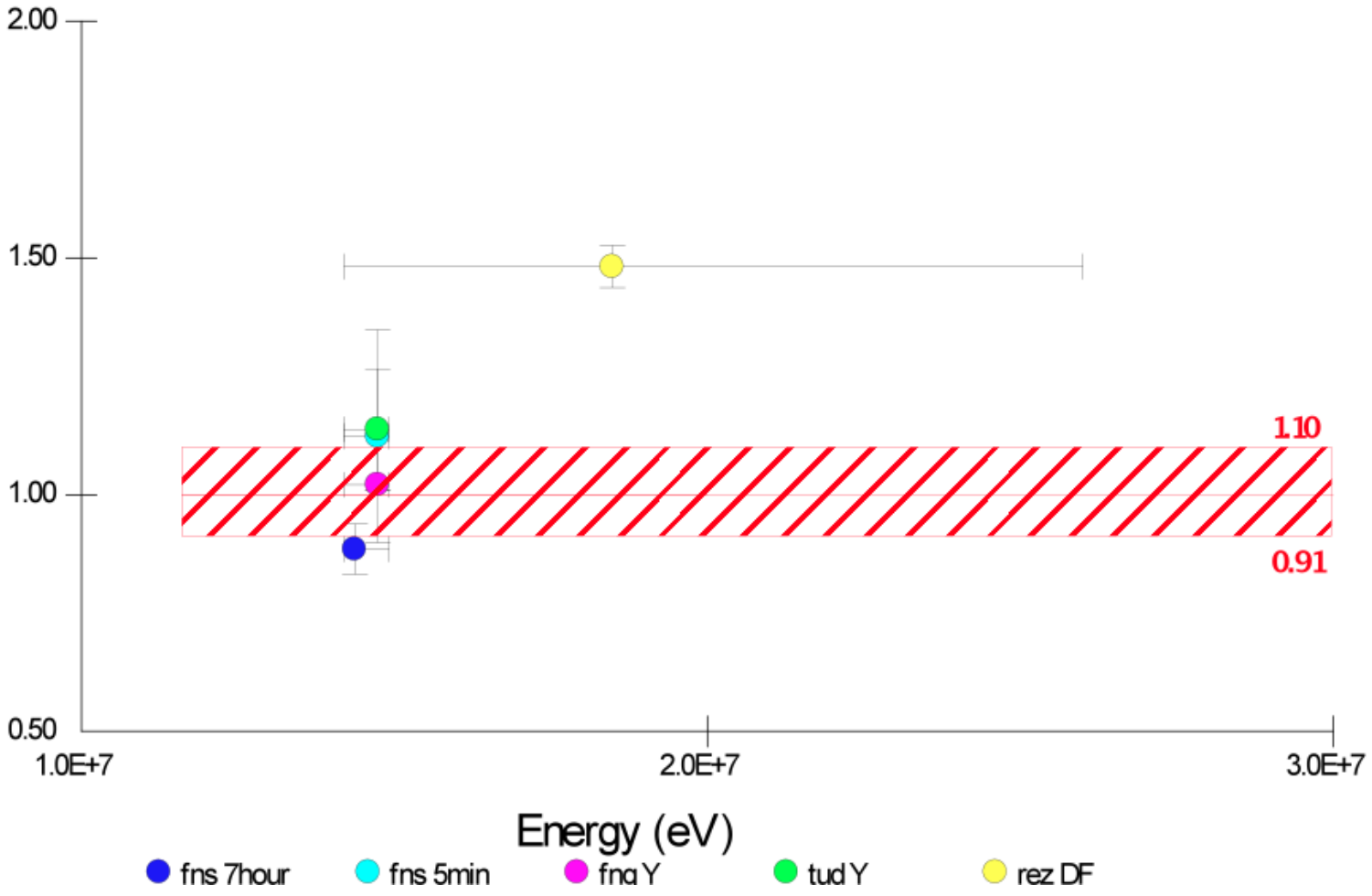
Extended C/E Integral – $^{89}Y(n,2n)^{88}Y$



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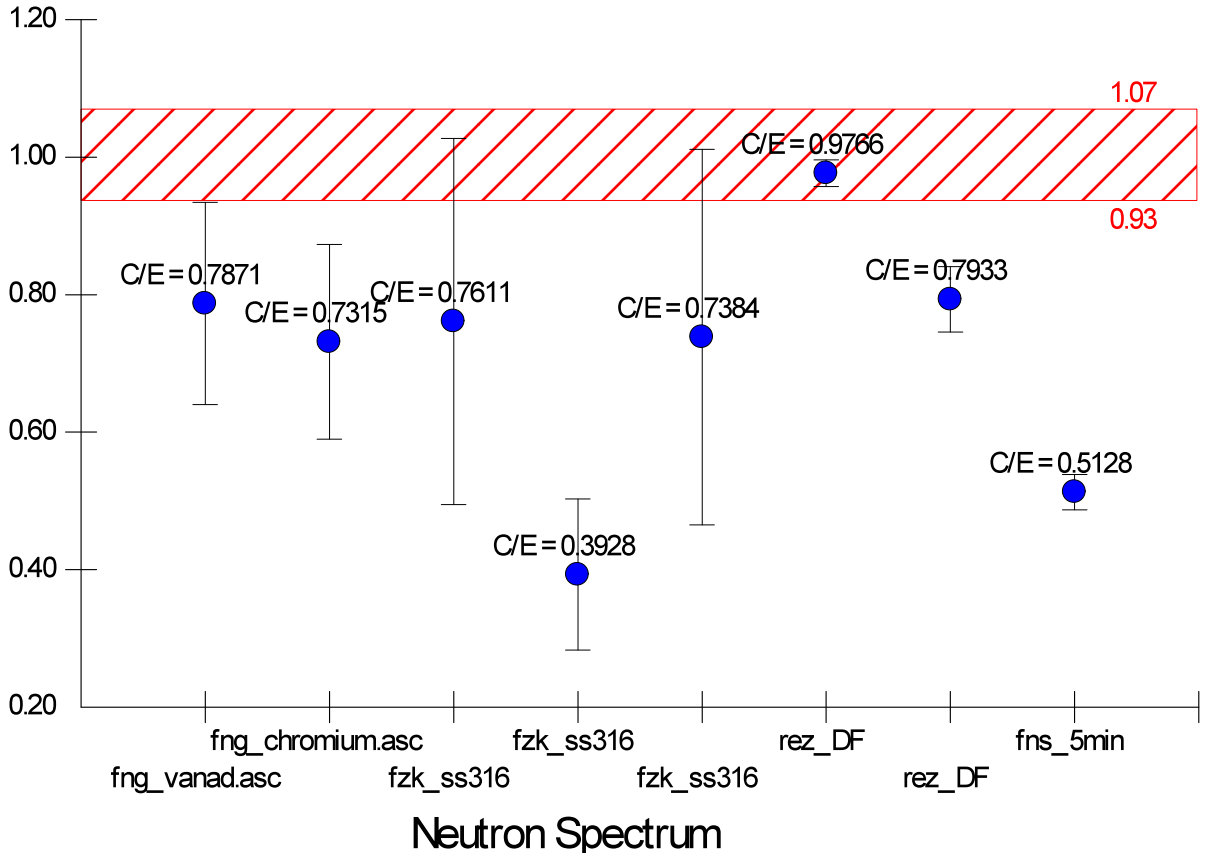
Reactions with score 5 – $^{50}Cr(n,2n)^{49}Cr$



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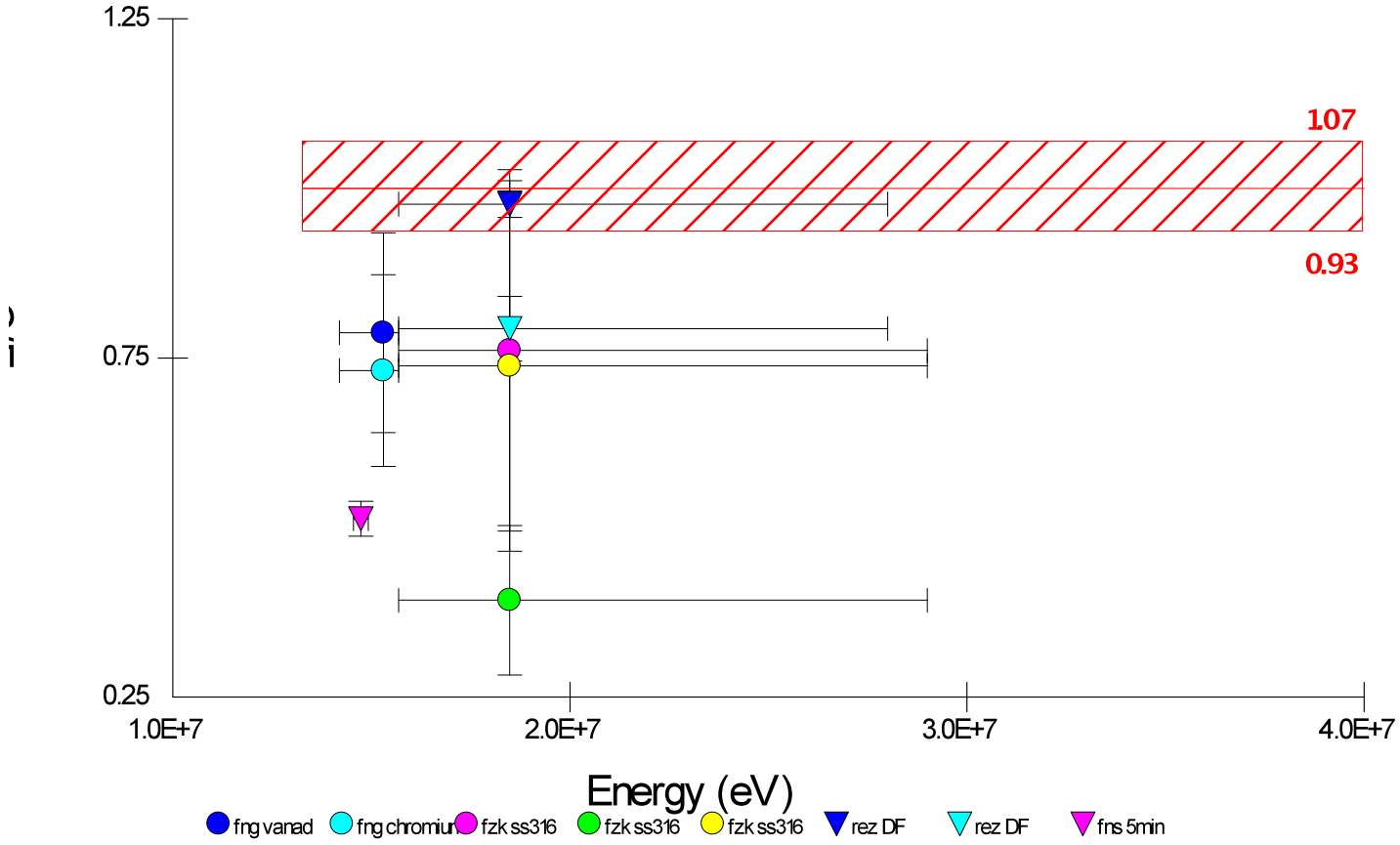
Extended C/E integral – $^{50}Cr(n,2n)^{49}Cr$



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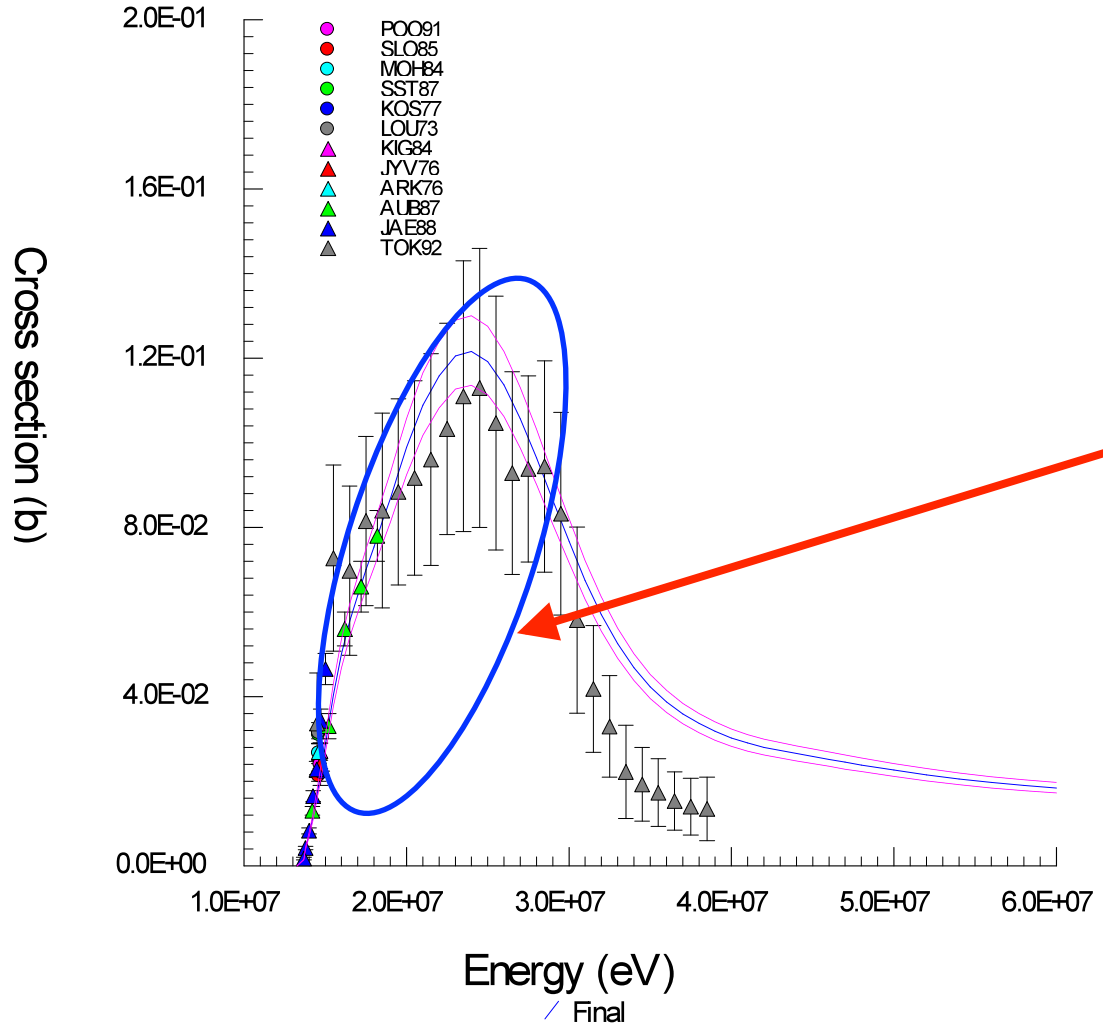
Reactions with score 5 - $^{50}Cr(n,2n)^{49}Cr$



Difficult to see how EAF values could be increased by ~ 30% to agree with integral

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EASY-2007/2010 validation

- *Validation of EASY-2001, -2003, -2005*
- *'Validation of EASY-2007 using integral measurements'*, **UKAEA FUS 547, 2007**
- All reports available from CCFE web site for download
- 564 pages, graphical report
- Materials:
  - All of EASY-2007 database
  - Re, Sn from FNG; - Er, La from TUD
  - Cr from Řež; - Y, Mo, Ta from FNG re-analysed
  - JAERI FNS measurements re-analysed
- Use of extended (energy dependent) C/E plot
- **470** reactions plotted, **217** validated

Apply to n-FENDL-3.0/A validation

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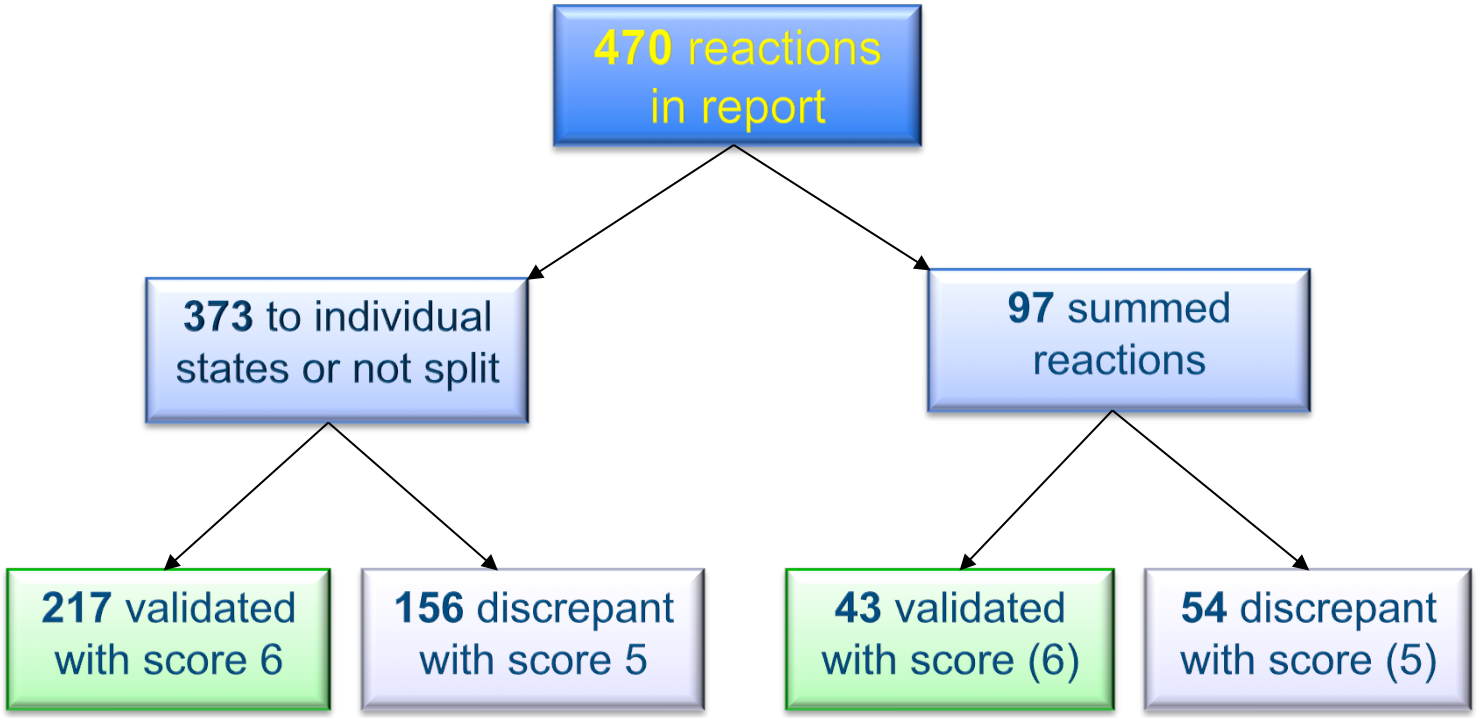
Summary

- Large database of integral data, many materials
- EASY approach, C/E for nuclide → C/E for reaction
- Use integral + differential data → Quality score
- Results for EASY-2007/2010 == FENDL-3.0/A



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d-, p-FENDL-3.0/A

- Assembled from EAF-2007 proton and deuteron induced activation-transmutation libraries
- Improved deuteron channels from the National Institute of Physics and Nuclear Engineering, Bucarest: Cu, Al..
- The deuteron-induced library contains data for 66,864 reactions, while the proton-induced library contains data for 67,925 reactions.
- Released to the IAEA in EAF pointwise data format with no uncertainty

Conclusions

- All aspects to assemble, process, verify and validate modern transport activation-transmutation file have been outlined. It Includes file format, numerical and physical contents, each processing sequences, intermediary steps, all processing codes used, leading to a file in ENDF-6 format that can be transformed into useful forms.
- Every individual steps have already been achieved

The Autumn of 2011 is seeing the birth of a new generation of nuclear data files feeding in new generation of activation-transmutation codes