Minor *Fe* isotopes

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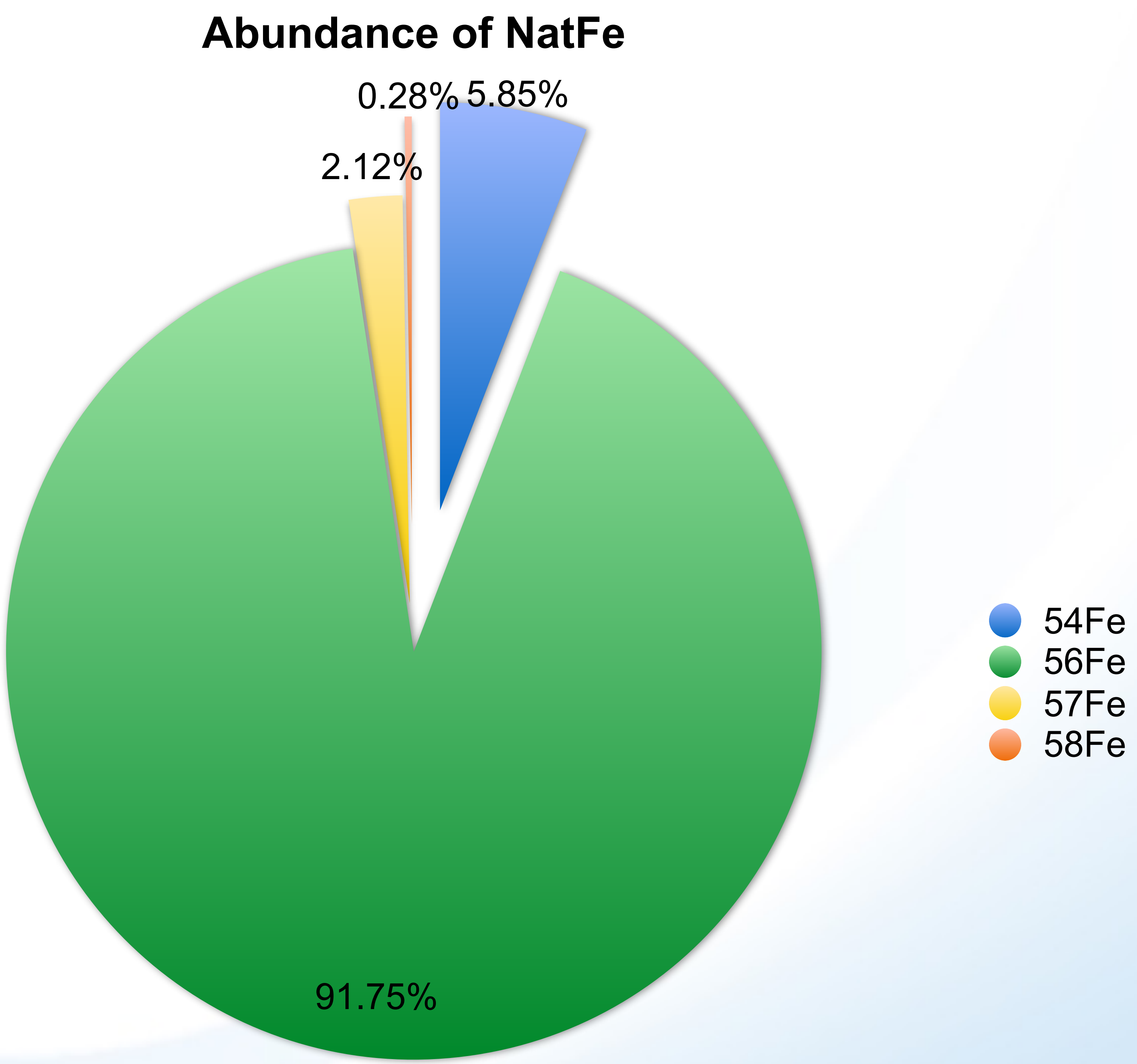
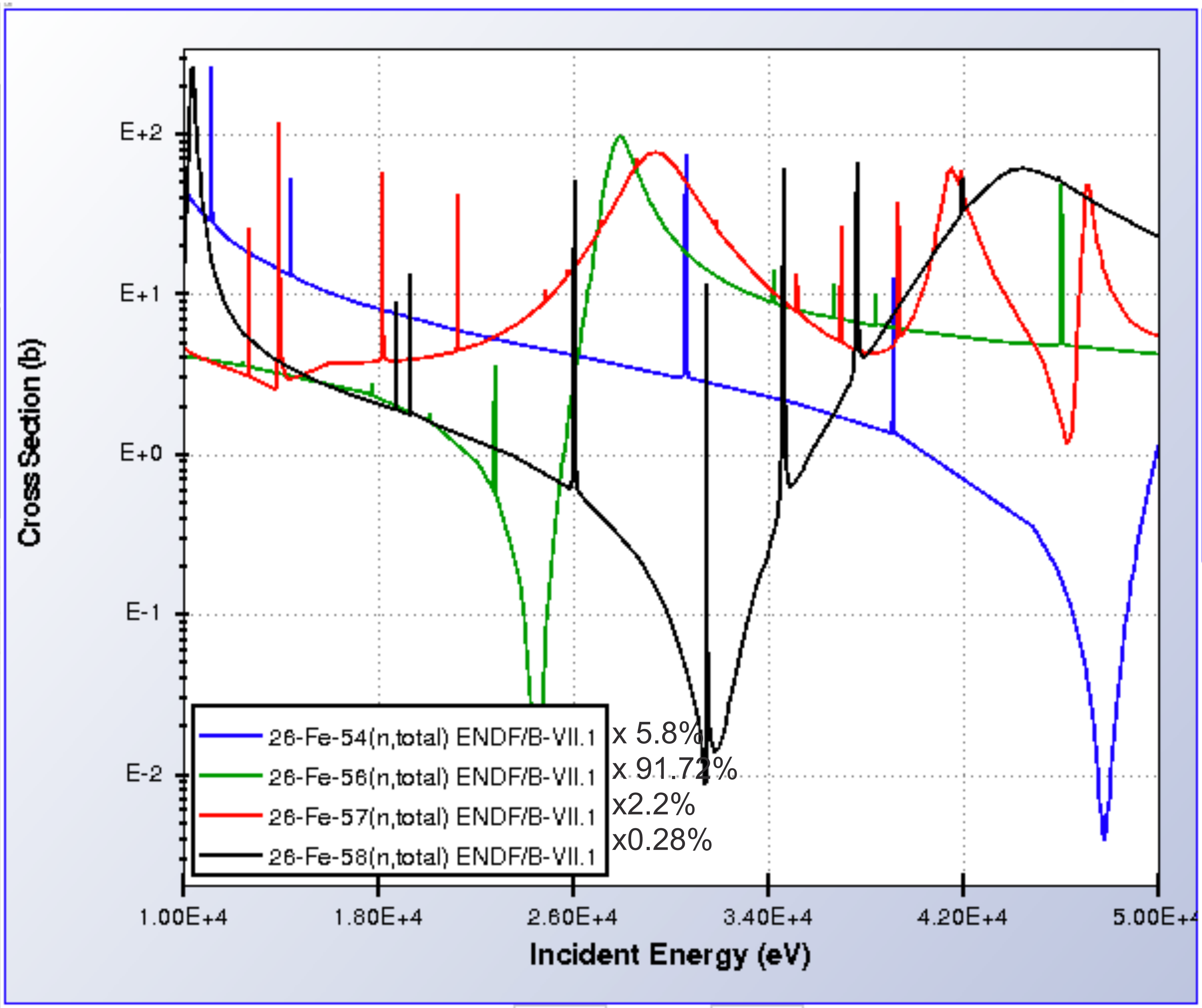
Mini-CSEWG 2016, April 11th – 12th, 2016

On the face of it, minor Fe isotopes should be unimportant



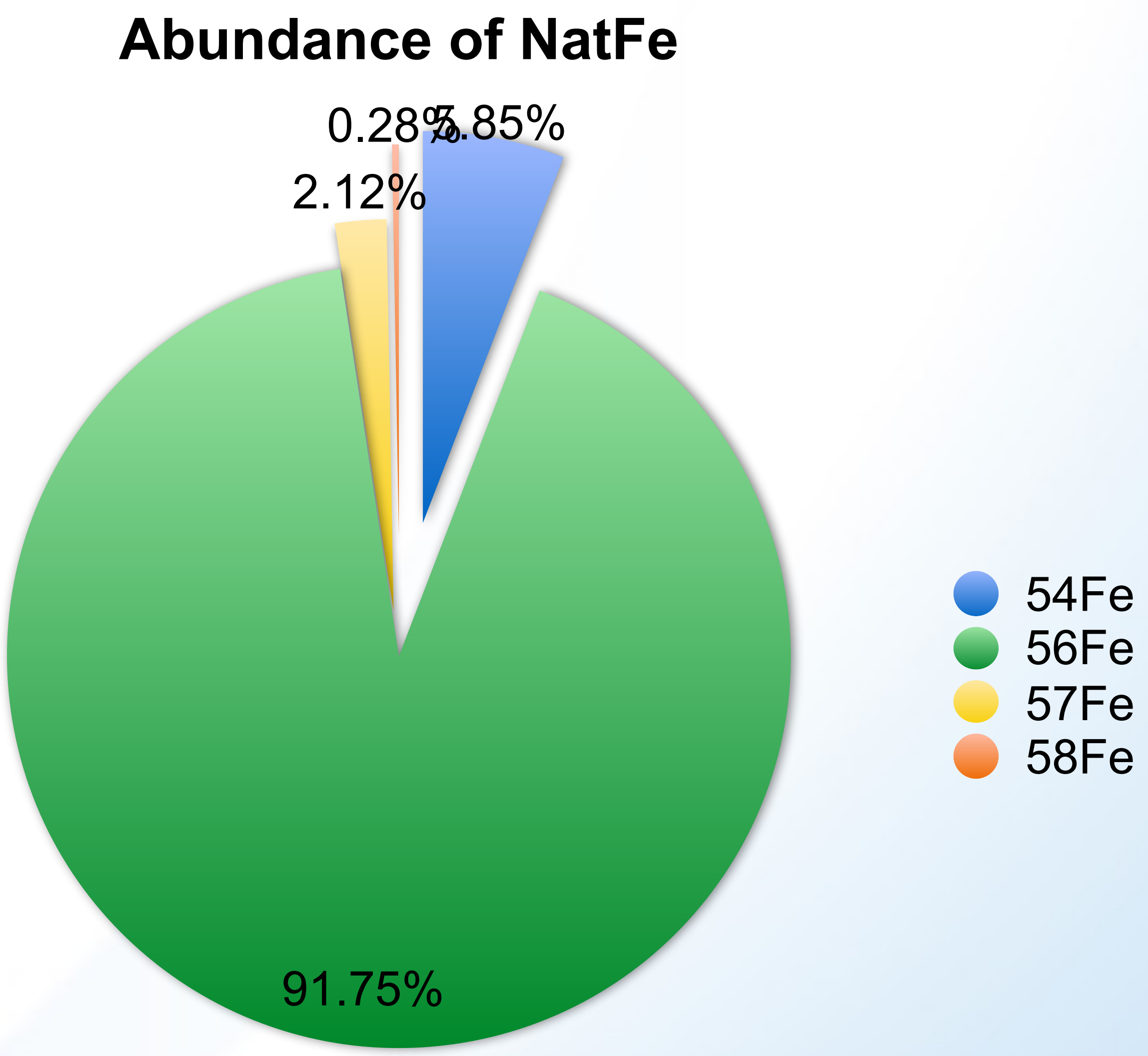
Minor Fe isotopes may play outsized role in some nuclear systems, especially systems used to validate 56Fe



Minor isotopes

Fast

- CC for incident/outgoing channels + DWBA
- Soukhovitskii and Capote dispersive OMP
- Gilbert-Cameron level densities
- Consistency among level-density parameters



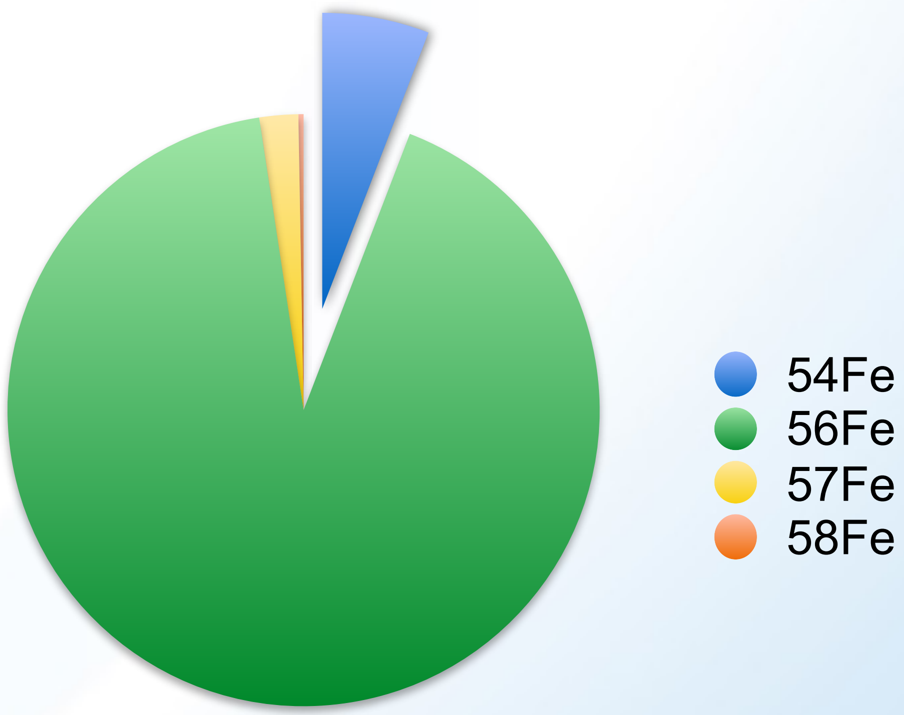
Resonances

- Adopted from either Atlas or Moxon (58Fe)
- Occasional tweaks

^{54}Fe

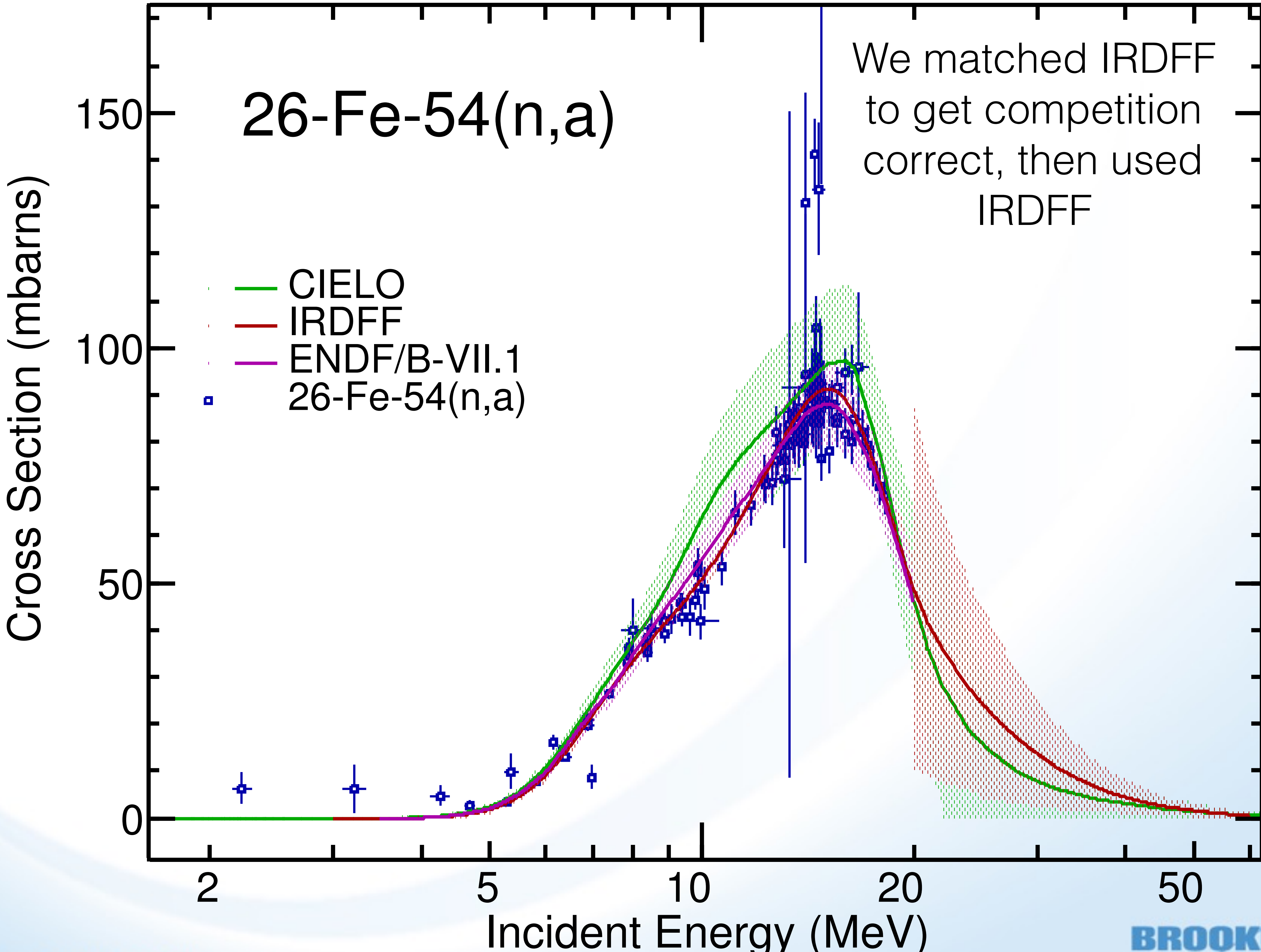
Fast

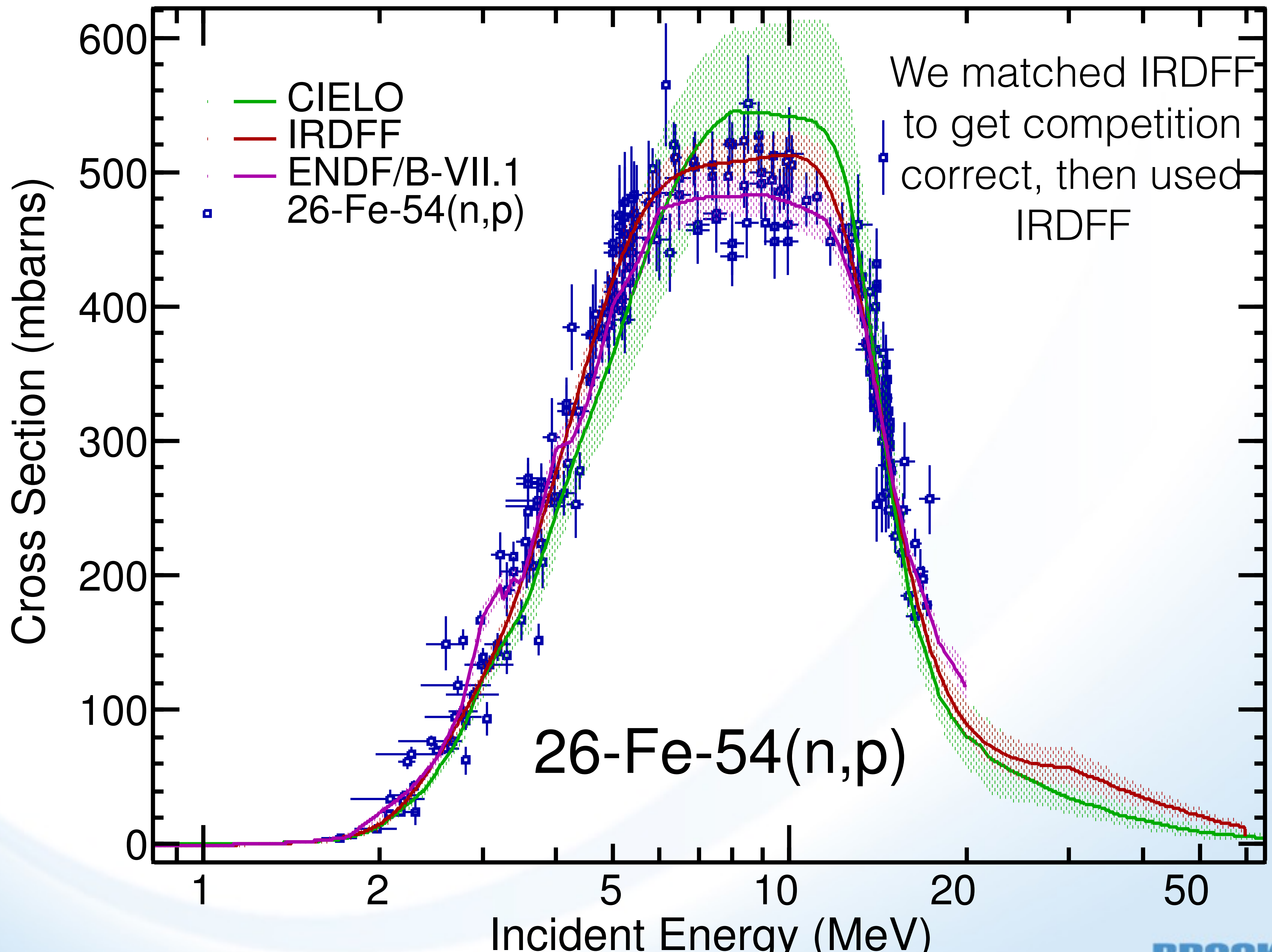
- Same Soukhovitskii and Capote dispersive OMP
- Same energy-dependent reduction of (n,tot) up to 3 MeV
- Fitted new LD parameters to (n,p), (n,2n) and (n,α) to dosimetry (IRDFF)
- Kept pre-equilibrium parameters within reasonable range
- Fitted deformation of DWBA levels to fill gap in double-differential neutron spectra

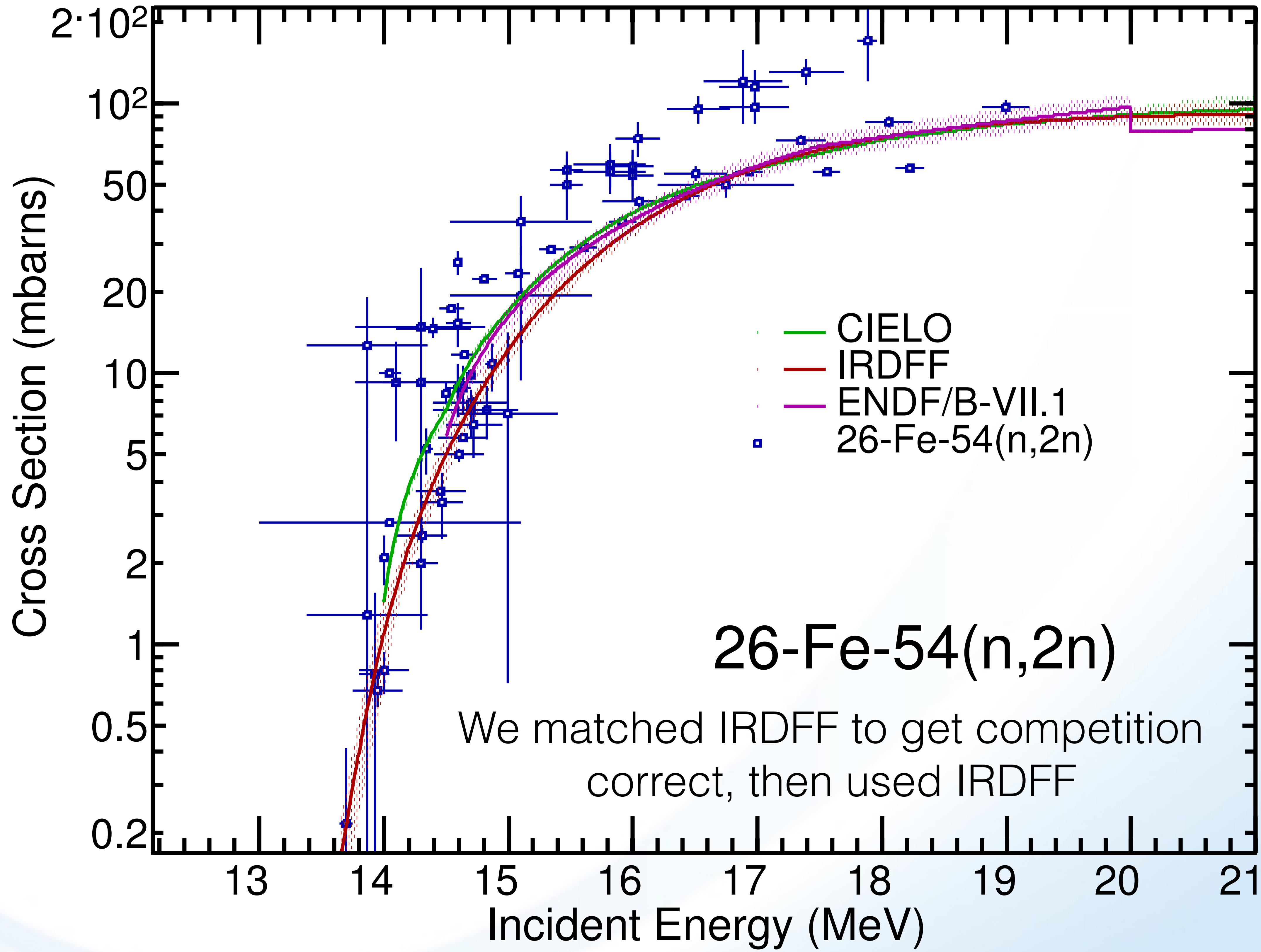


Resonances

- From Atlas, but converted from MLBW to RM, then tweaked

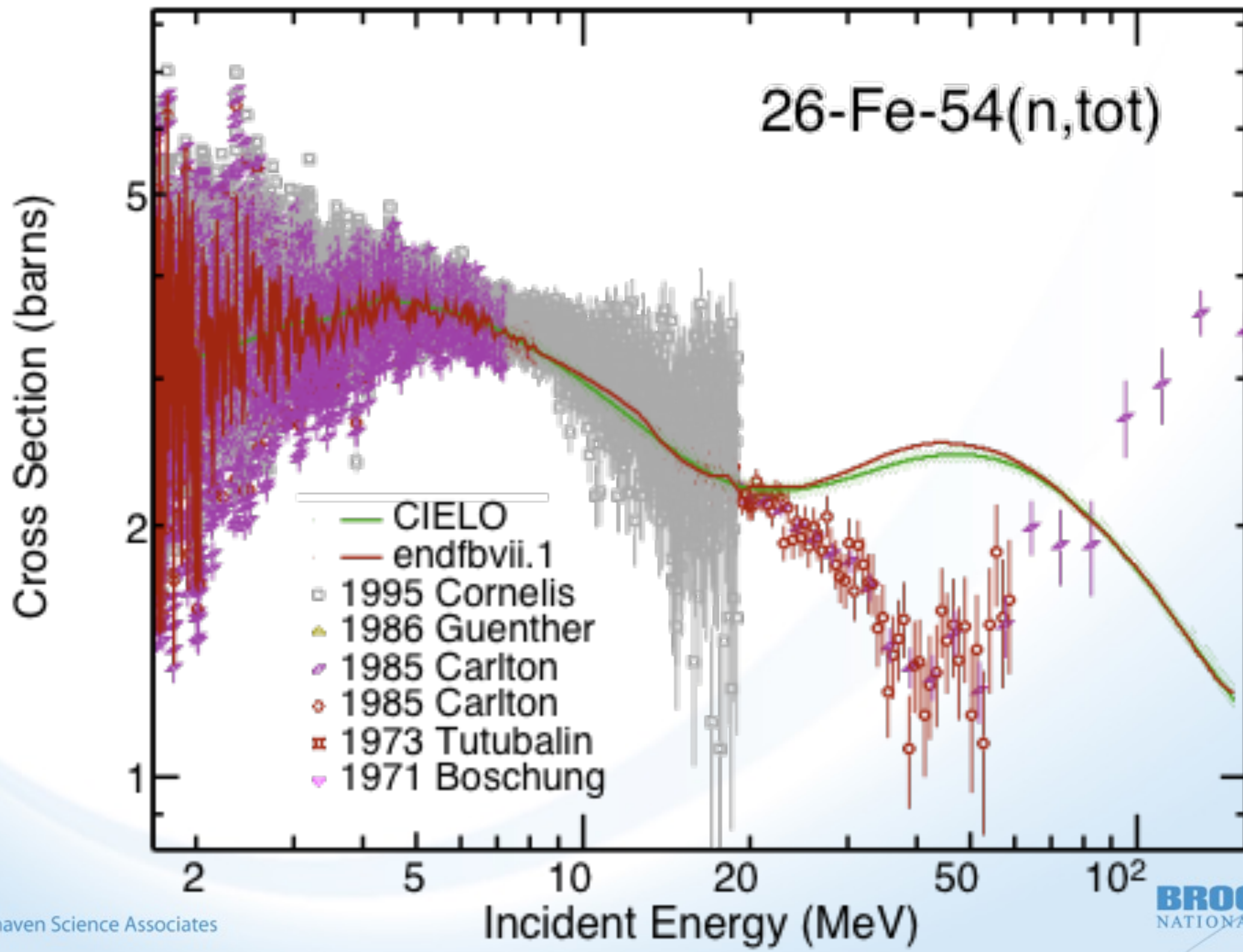

26-Fe-54(n,a)
We matched IRDFF to get competition correct, then used IRDFF
CIELO
IRDFF
ENDF/B-VII.1
26-Fe-54(n,a)
Cross Section (mbarns)
150
100
50
0
2
5
10
20
50
Incident Energy (MeV)


Cross Section (mbarns)
600
500
400
300
200
100
0
1
2
5
10
20
50
Incident Energy (MeV)
CIELO
IRDFF
ENDF/B-VII.1
26-Fe-54(n,p)
We matched IRDFF to get competition correct, then used IRDFF
26-Fe-54(n,p)

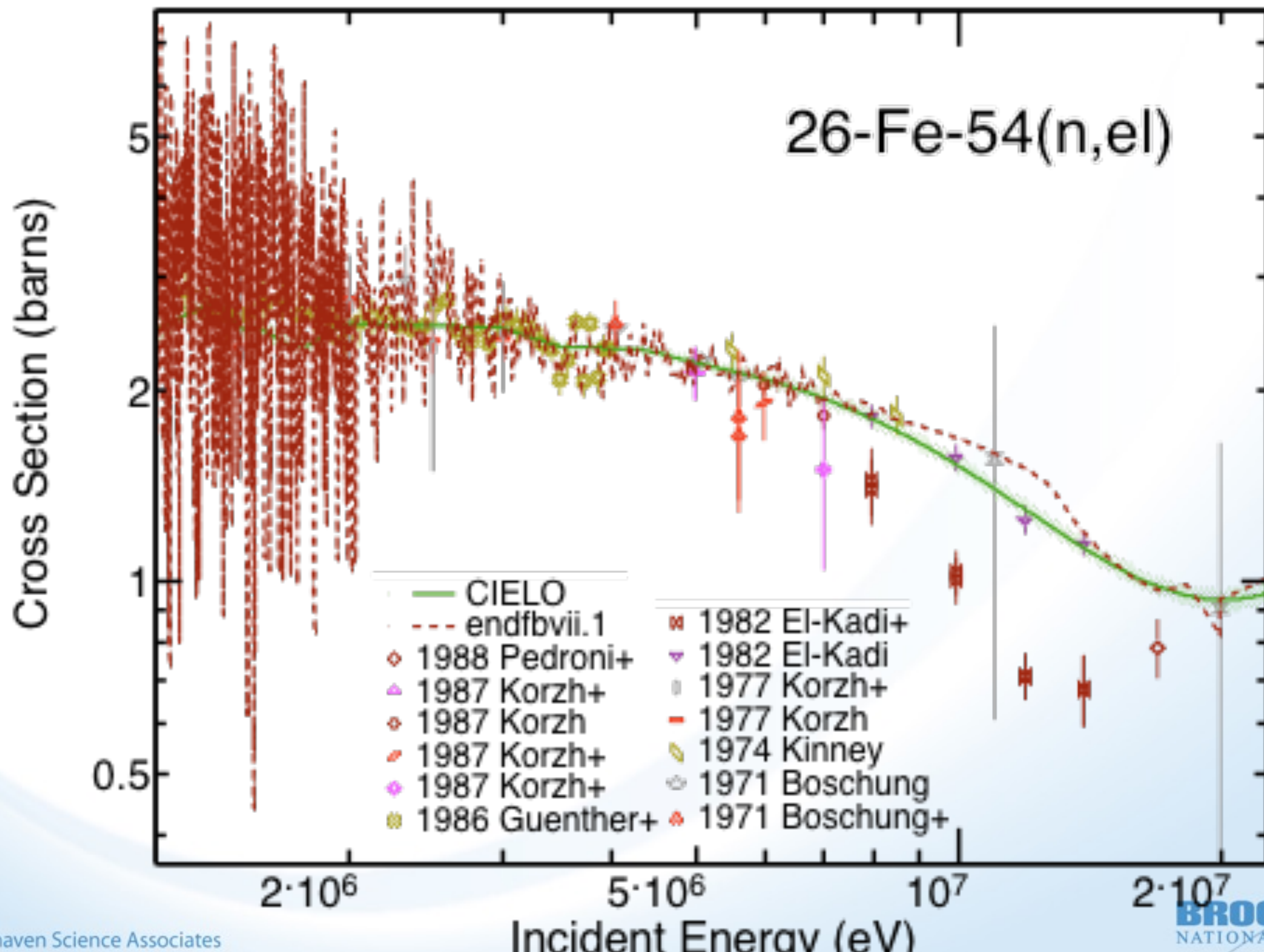


2·10²
10²
50
20
10
5
2
1
0.5
0.2
Cross Section (mbarns)
13
14
15
16
17
18
19
20
21
Incident Energy (MeV)
CIELO
IRDFF
ENDF/B-VII.1
26-Fe-54(n,2n)
26-Fe-54(n,2n)
We matched IRDFF to get competition correct, then used IRDFF

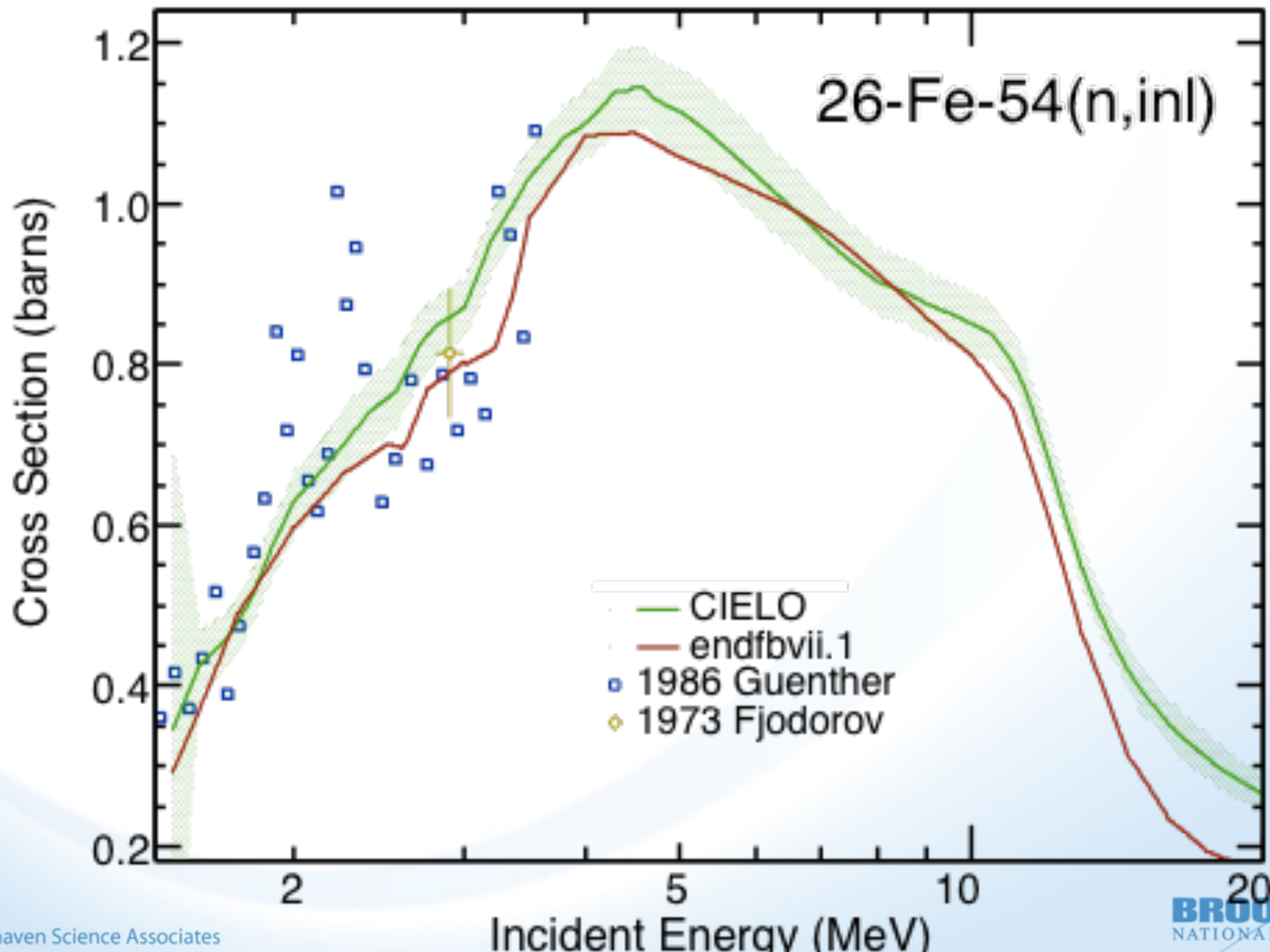
^{54}Fe


26-Fe-54(n,tot)
Cross Section (barns)
Incident Energy (MeV)
5
2
1
2
5
10
20
50
10^2
CIELO
endfbvii.1
1995 Cornelis
1986 Guenther
1985 Carlton
1985 Carlton
1973 Tutubalin
1971 Boschung

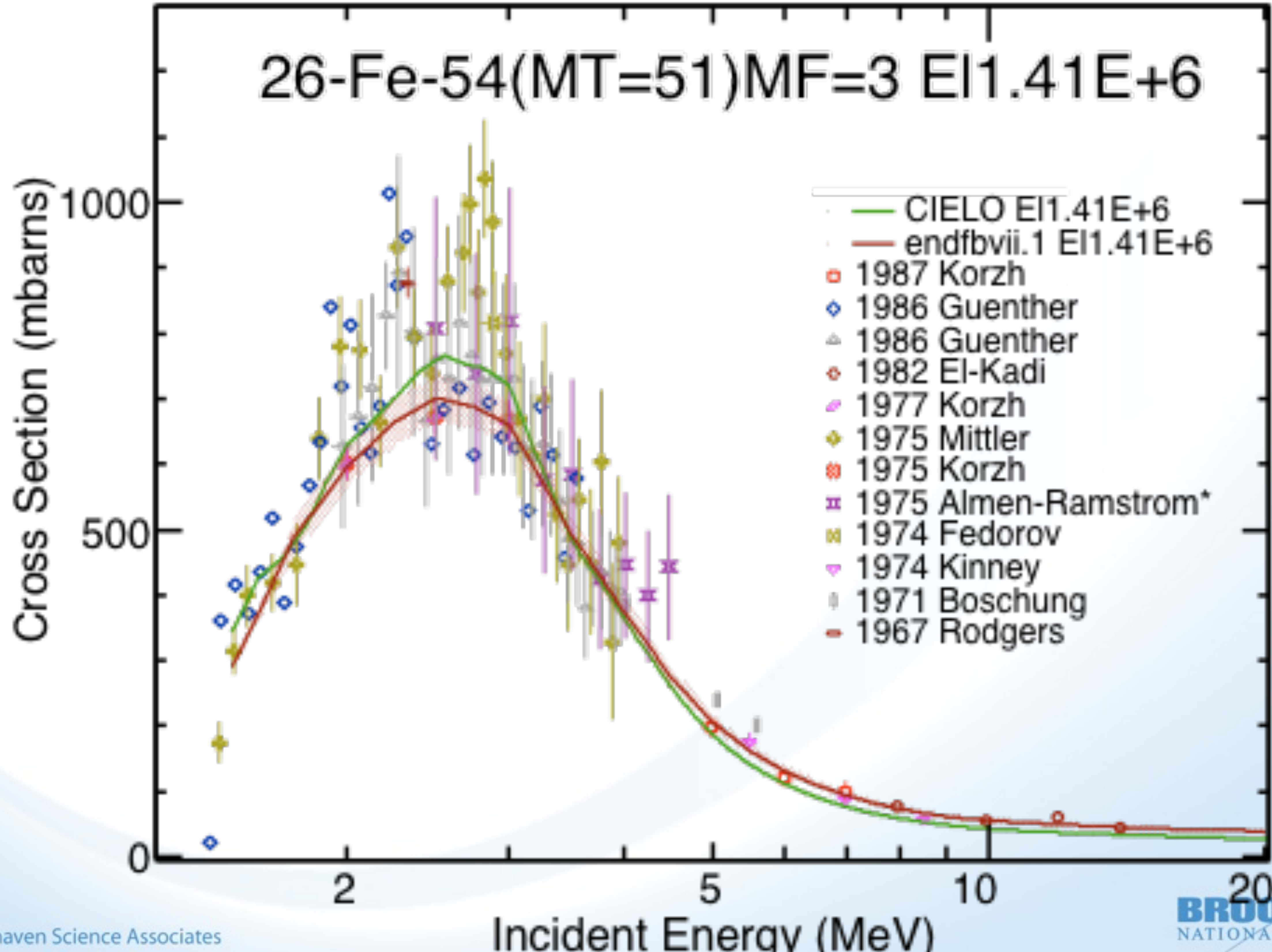
^{54}Fe


26-Fe-54(n,el)
Cross Section (barns)
Incident Energy (eV)
5
2
1
0.5
2·10^6
5·10^6
10^7
2·10^7
CIELO
endfbvii.1
1988 Pedroni+
1987 Korzh+
1987 Korzh
1987 Korzh+
1987 Korzh+
1986 Guenther+
1982 El-Kadi+
1982 El-Kadi
1977 Korzh+
1977 Korzh
1974 Kinney
1971 Boschung
1971 Boschung+

^{54}Fe

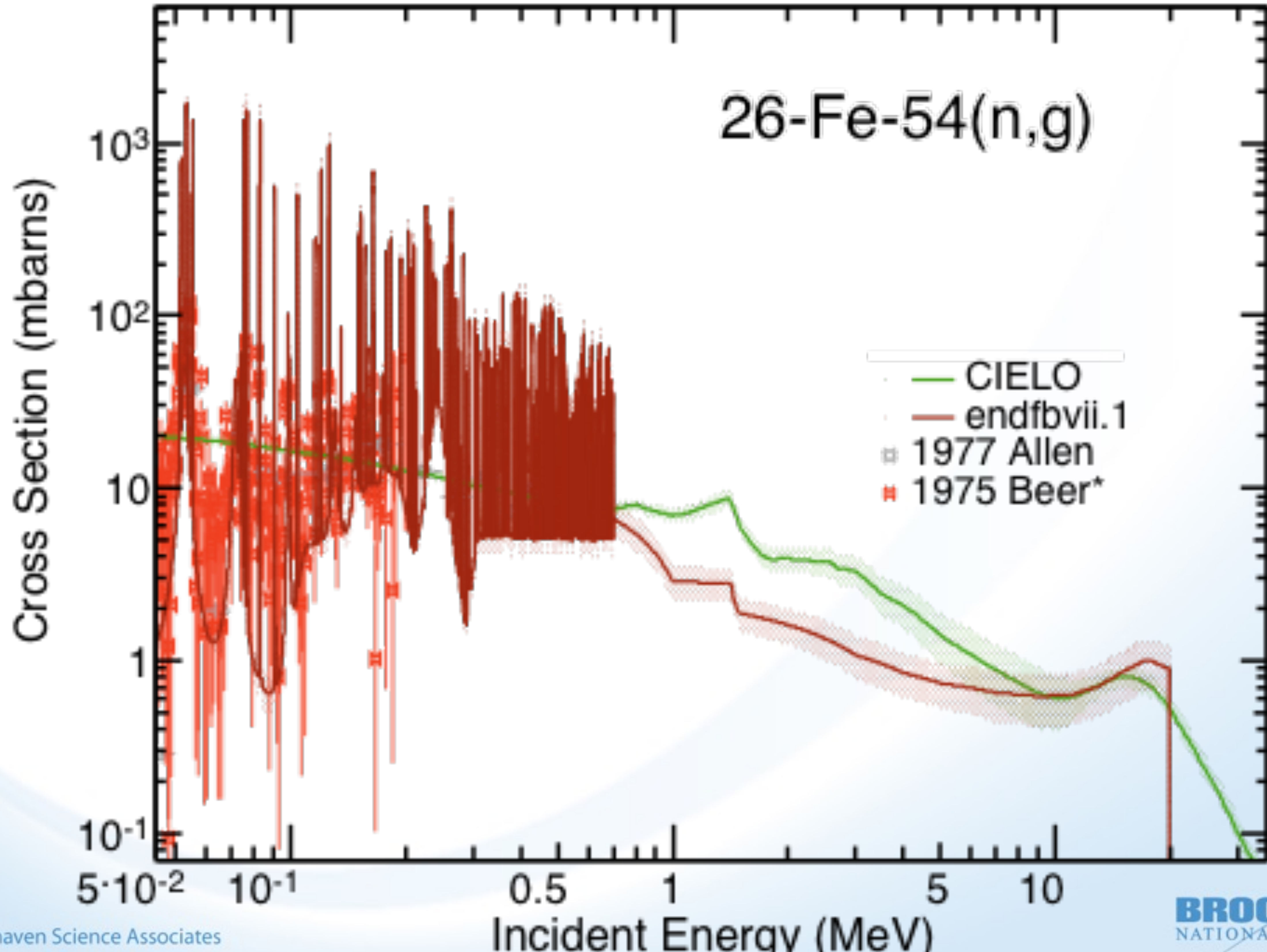

26-Fe-54(n,inl)
Cross Section (barns)
Incident Energy (MeV)
1.2
1.0
0.8
0.6
0.4
0.2
2
5
10
20
CIELO
endfbvii.1
1986 Guenther
1973 Fjodorov

^{54}Fe



26-Fe-54(MT=51)MF=3 El1.41E+6
Cross Section (mbarns)
1000
500
0
2
5
10
20
Incident Energy (MeV)
CIELO El1.41E+6
endfbvii.1 El1.41E+6
1987 Korzh
1986 Guenther
1986 Guenther
1982 El-Kadi
1977 Korzh
1975 Mittler
1975 Korzh
1975 Almen-Ramstrom*
1974 Fedorov
1974 Kinney
1971 Boschung
1967 Rodgers

^{54}Fe

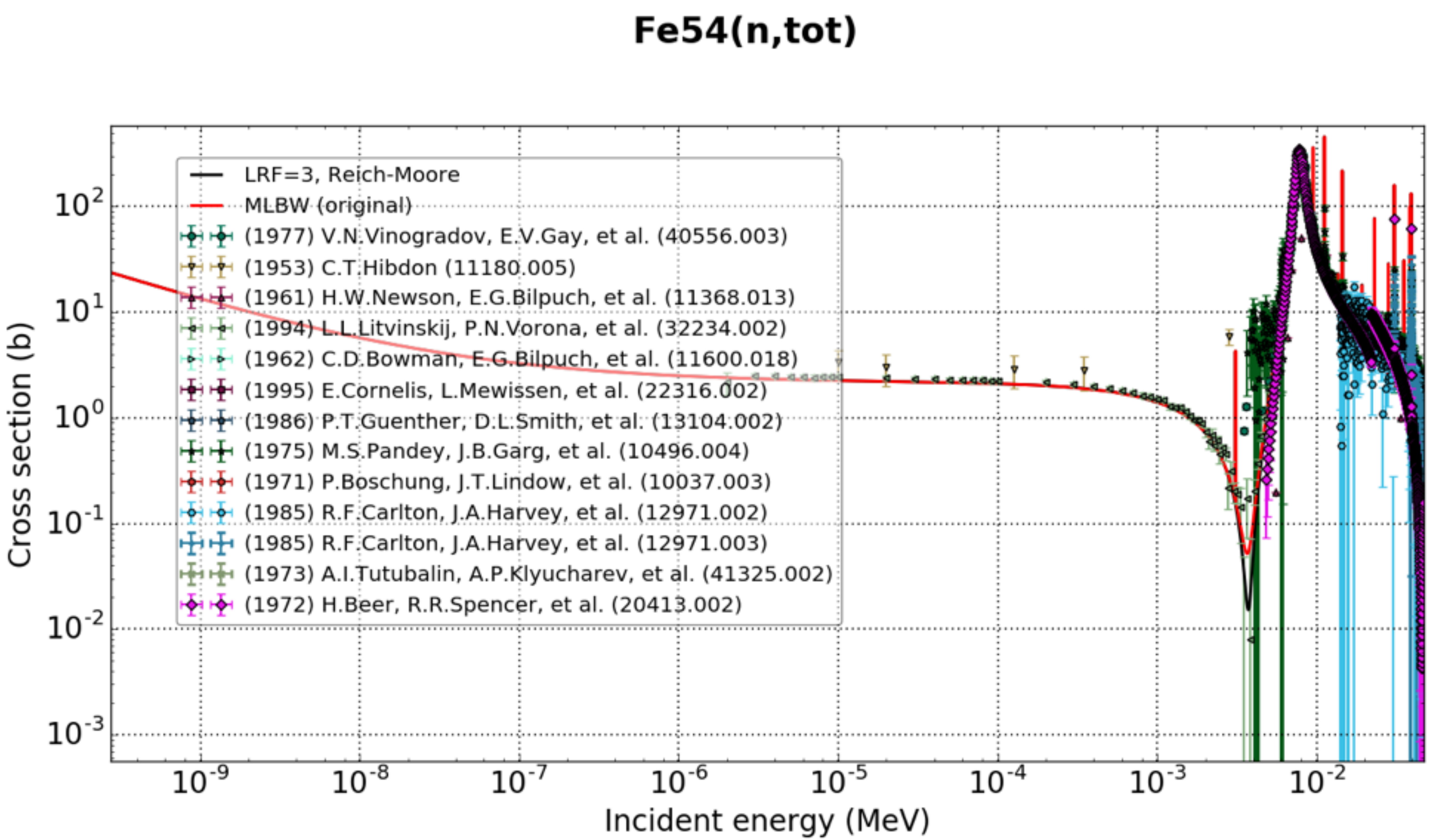

26-Fe-54(n,g)
Cross Section (mbarns)
10³
10²
10
1
10⁻¹
5·10⁻²
10⁻¹
0.5
1
5
10
Incident Energy (MeV)
CIELO
endfbvii.1
1977 Allen
1975 Beer*

^{54}Fe: from new Atlas, but in RM

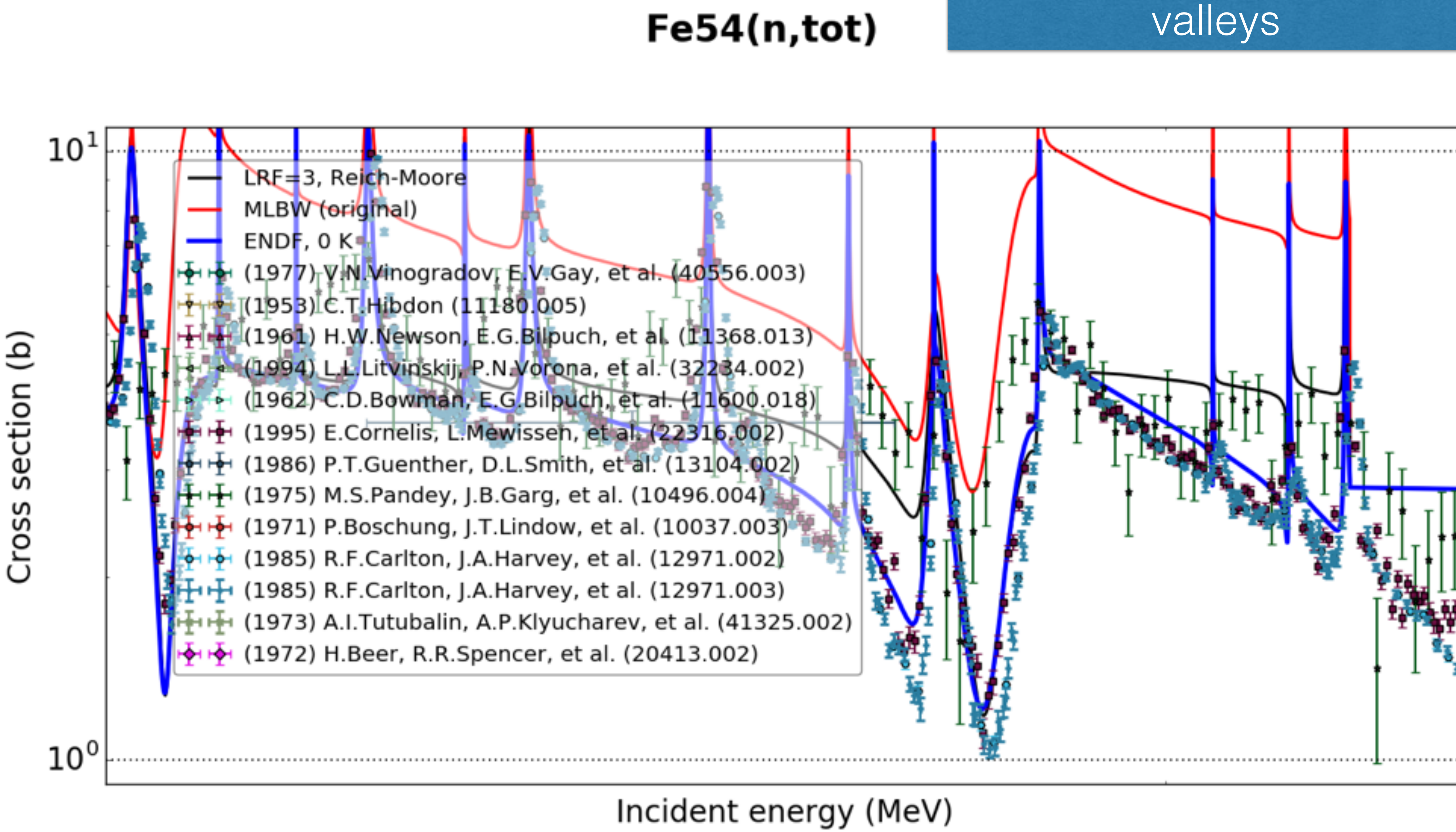
- **Convert MLBW (LRF=2) to Reich Moore (LRF=3)**
  - improved interference minima, but messed up thermal
- **Added/adjusted fictitious strong levels to fix thermal cross section**
- **Imposed fictitious strong levels above E_{max} to get better interference effects and improve agreement with total cross section data**

		Before			After		
E_R (keV)	L	J	Γ_γ (eV)	Γ_n (eV)	J	Γ_γ (eV)	Γ_n (eV)
-1223.3	**0**	n/a	n/a	n/a	**1/2**	**1.0**	**64,062**
-22.24 -> **-20.499**	0	1/2	1.55	8474	1/2	1.55	**6872**
740.56	2	**1/2**	0.96	386.5	**3/2**	0.96	386.5
741.44	2	**1/2**	0.96	424	**3/2**	0.96	424
814.627368	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**1508.68838**
815.801766	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**4148.82574**
824.106211	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**3848.05147**
833.931452	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**5844.58959**
847.326171	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**5565.40352**
1000	**0**	n/a	n/a	n/a	**1/2**	**4.0**	**26,000**

Tweaks of bound levels get low energy part correct



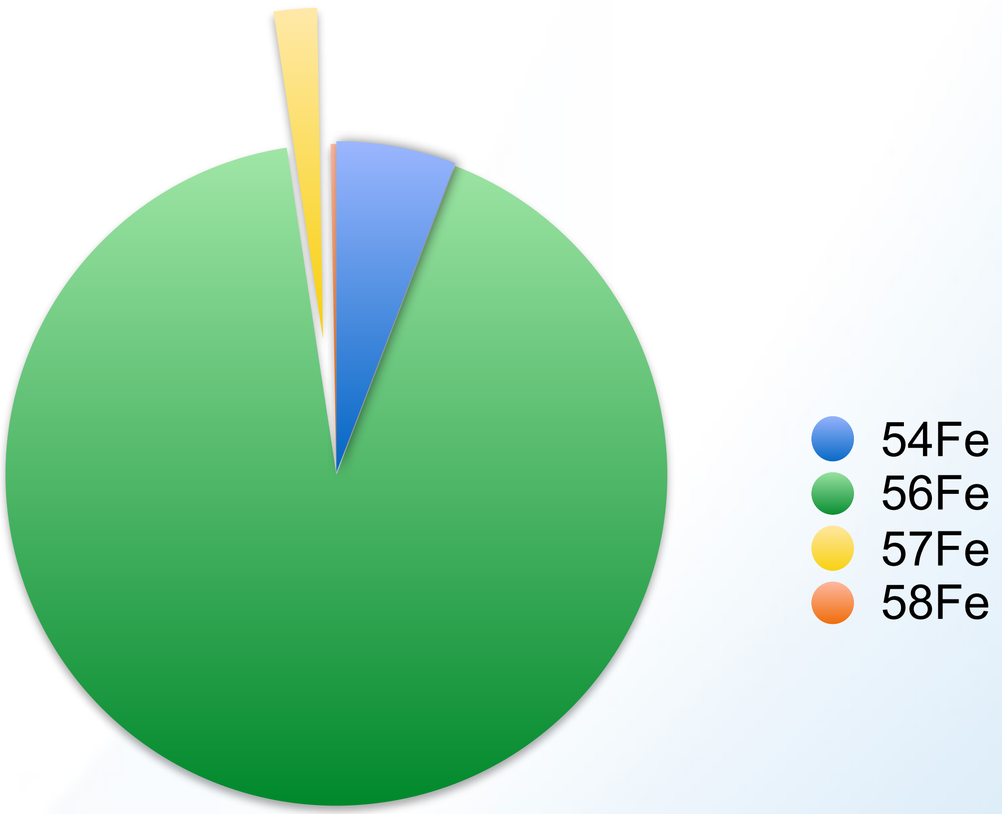
Added a cluster of high energy S-wave resonances to interfere at the upper end and pull down the valleys



^{57}Fe

Fast

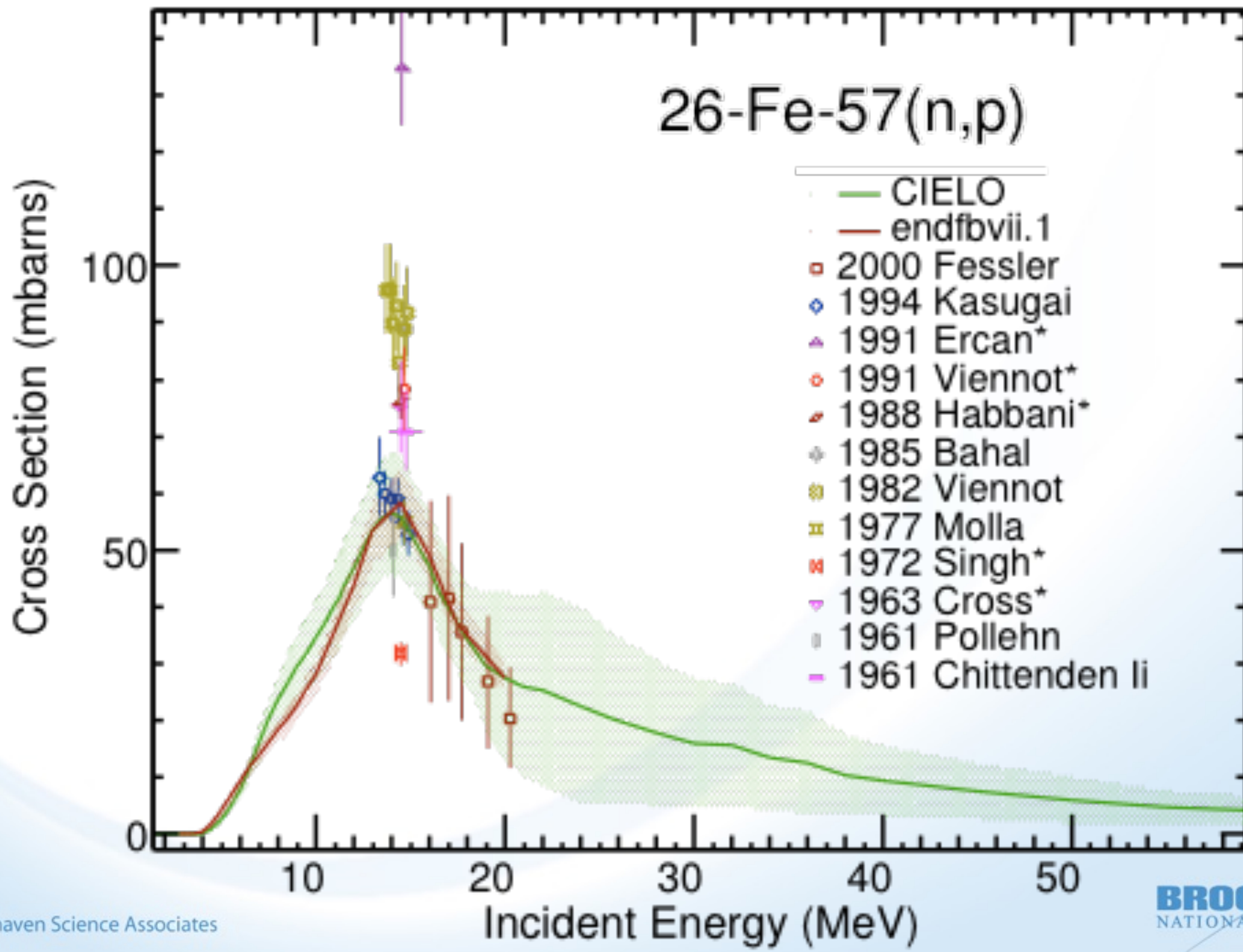
- Soukhovitskii-Capote OMP for odd iron isotopes
- No reduction of (n,tot) necessary
- Few experimental datasets (No dosimetry file)
- Fit (n,p) to select experiments
- Low-energy peak for inelastic cross section



Resonances

- From Atlas, with extensive modifications
- Converted from MLBW to LRF=7

^{57}Fe



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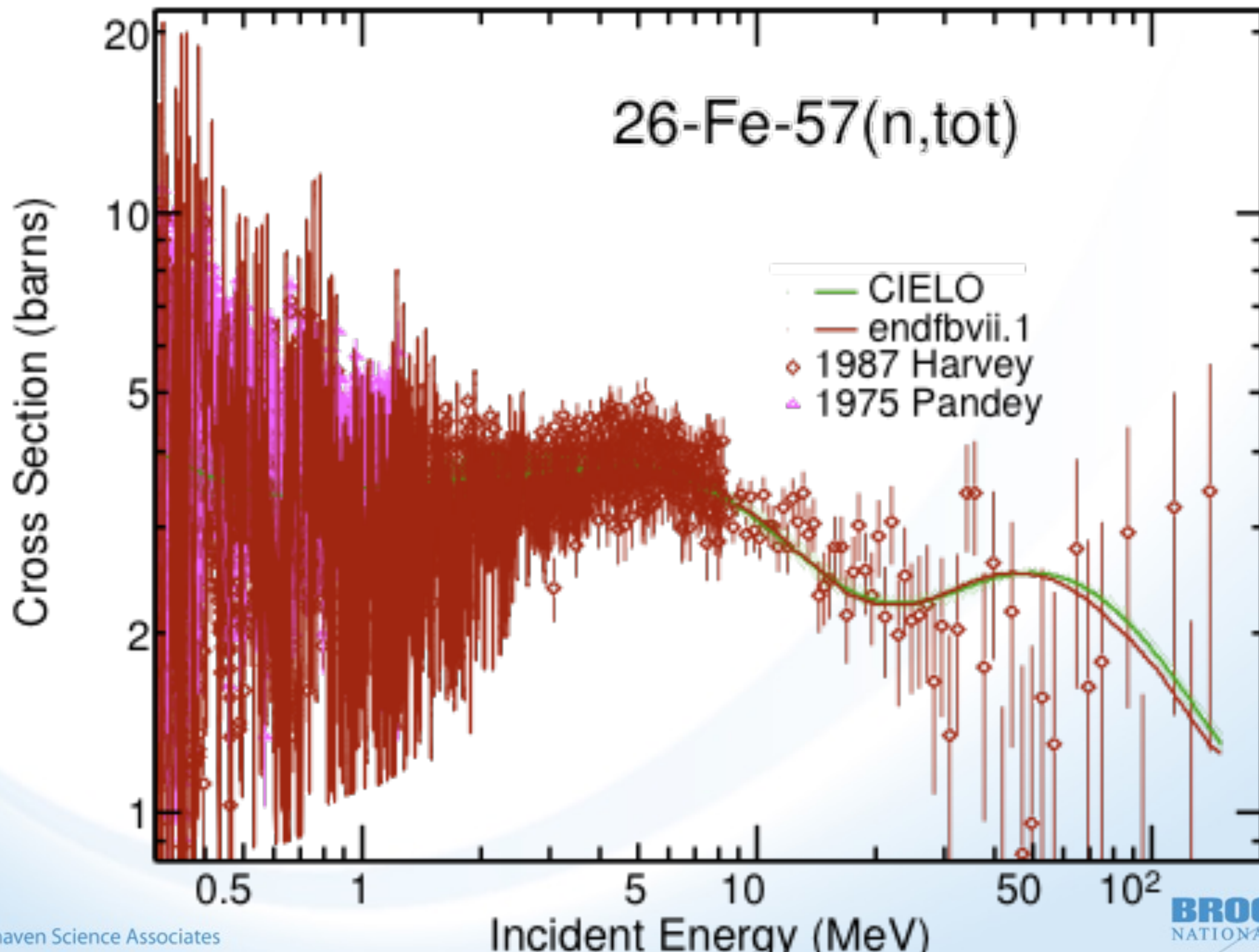
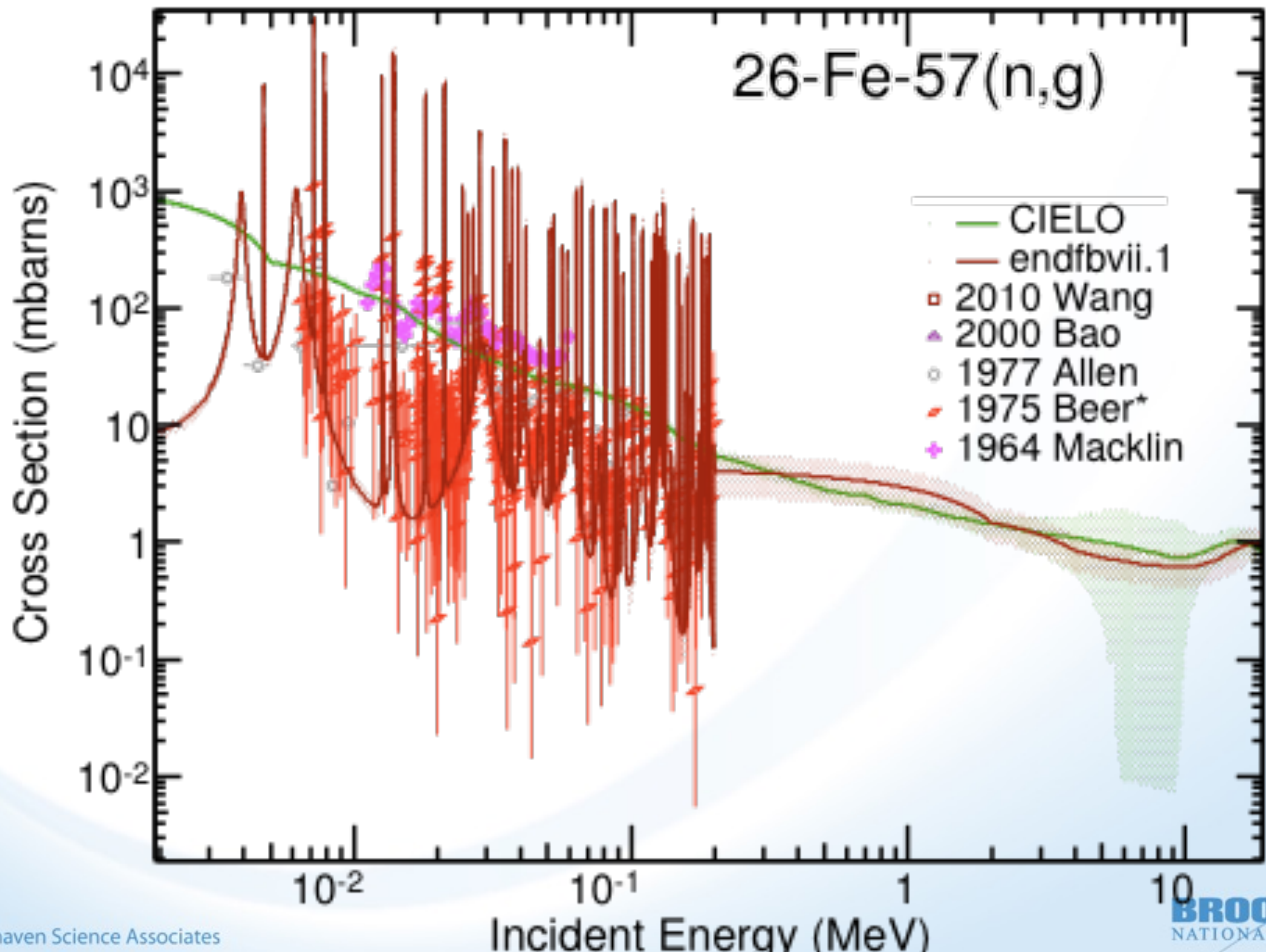
^{57}Fe


26-Fe-57(n,tot)
CIELO
endfbvii.1
1987 Harvey
1975 Pandey
Cross Section (barns)
Incident Energy (MeV)
20
10
5
2
1
0.5
1
5
10
50
10^2

^{57}Fe



26-Fe-57(n,g)
CIELO
endfbvii.1
2010 Wang
2000 Bao
1977 Allen
1975 Beer*
1964 Macklin
Cross Section (mbarns)
Incident Energy (MeV)
10⁴
10³
10²
10
1
10-1
10-2
10-2
10-1
1
10

^{57}Fe: from new Atlas, but converted to Reich-Moore (LRF=7)

- **Said's resonances given in MLBW formatted ENDF file with extra column containing (n,n') widths**
  - (n,tot), (n,el) and (n,g) widths based on Geel parameters, likely generated in Reich-Moore approximation
  - (n,n') resonances determined by subtracting capture resonances from (n,tot) where no (n,el) present
    - E_x = 14.410 keV
    - S wave only
    - Capture widths known only from area under resonance

- **MACS(30 keV)=42 mb, consistent with Bao's recommended value of 40 mb**
  - Switching to RM disturbs this result

- **Dave converted resonances into LRF=7 format and flipped the approximation flag to Reich-Moore, keeping resonance parameters (mostly) unchanged**

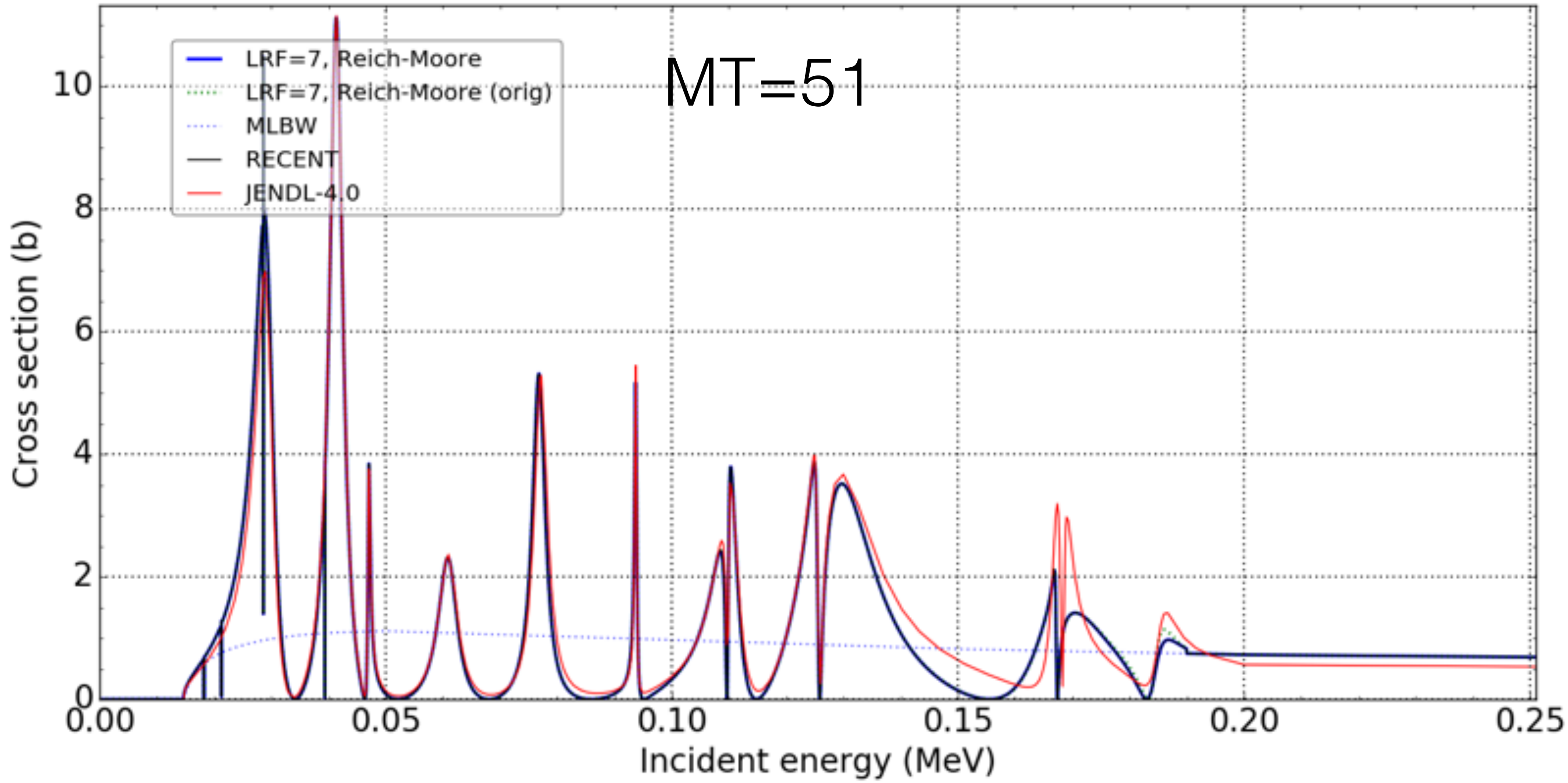
To our knowledge, this is first time an LRF=7 evaluation was produced without SAMMY

Therefore, peer review from Andrej Trkov and Red Cullen was essential

Red's major concerns

1. Have the background cross sections been correctly handled in all reactions? **YES**
2. Has potential scattering converged at the L specified in file? **YES**
3. Are there missing (L,J,S,MT) combinations from the channel specification? **YES!!!!!**
4. Are there missing s- or p- wave resonances? **PROBABLY!**
5. The valleys in the (n,tot) toward the upper end of the RRR are filled in in this evaluation? **FOR THE MOST PART**
6. Do we match the MACS(30 keV) value for capture? **YES**

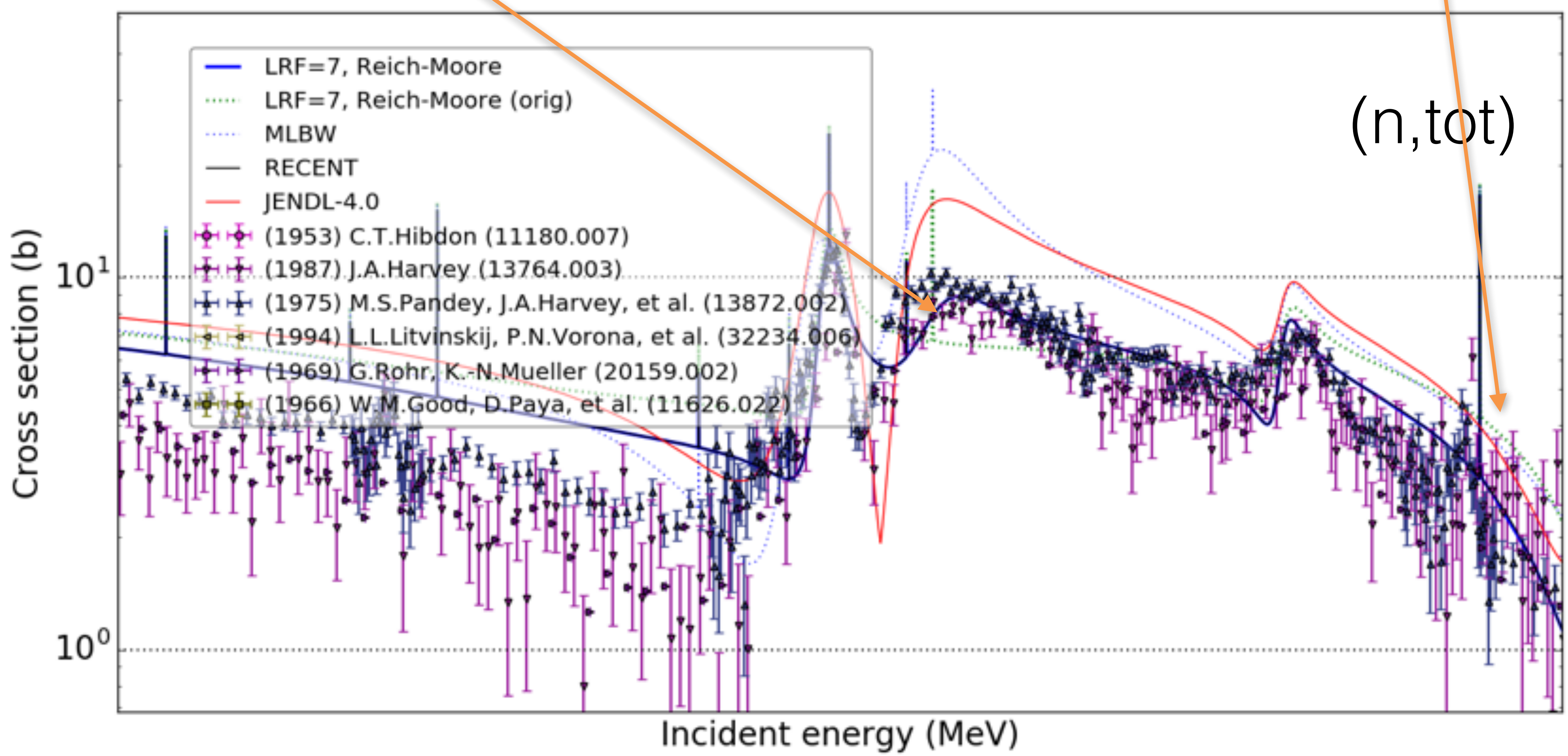
Widths determined from (n,tot) widths and capture area, all assumed S-wave



5. The valleys in the (n,tot) toward the upper end of the RRR are filled in

- Reworked near Ehi
  - add 4 s-wave above Ehi to get tails
  - add 1 s-wave at 169.31 keV to get interference

- tweak 3 resonances near 185 keV to get interference better



log scale on too coarse a grid, sorry!

5. The valleys in the (n,tot) toward the upper end of the RRR are filled in

		Before			After		
E_R (kev)	J	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)
169.31	0				1801.38	1800	1.38
176.30	0	701.20	700.00	1.20	501.20	500	1.20
185.00	1	3903.00	3500.00	3.00	5203.00	4800	3.00
189.50	0	3201.50	3200.00	1.50	4201.50	4200	1.50
194.25	0				703.55	700	3.55
197.30	0				702.57	700	2.57
198.90	0				701.18	700	1.18
200.10	0				700.99	700	0.99

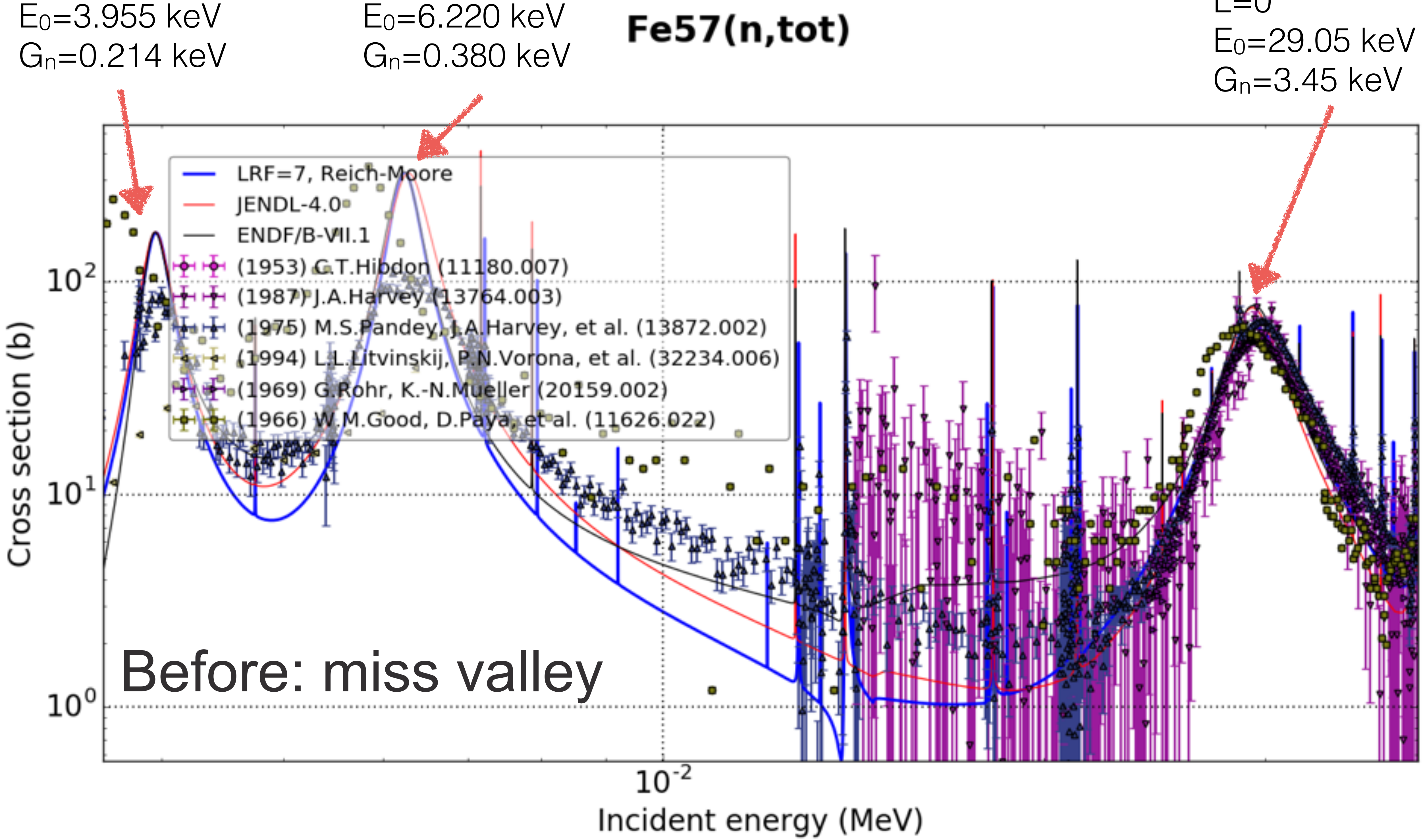
1) E_{hi}=190 keV; 2) Γ_γ determined from $g\Gamma_n\Gamma_\gamma/\Gamma$ assuming $g\Gamma_n/\Gamma$=0.253;
3) E_R=185 keV has MT51 resonance with $\Gamma_{n'}$=400 eV;
4) new resonances from Atlas with tuned Γ_n

5. The valleys in the (n,tot) near 25 keV live in "window" of 56Fe resonances

J^{Pi}=0+
L=0
E_0=3.955 keV
G_n=0.214 keV

J^{Pi}=1+
L=0
E_0=6.220 keV
G_n=0.380 keV

J^{Pi}=1+
L=0
E_0=29.05 keV
G_n=3.45 keV

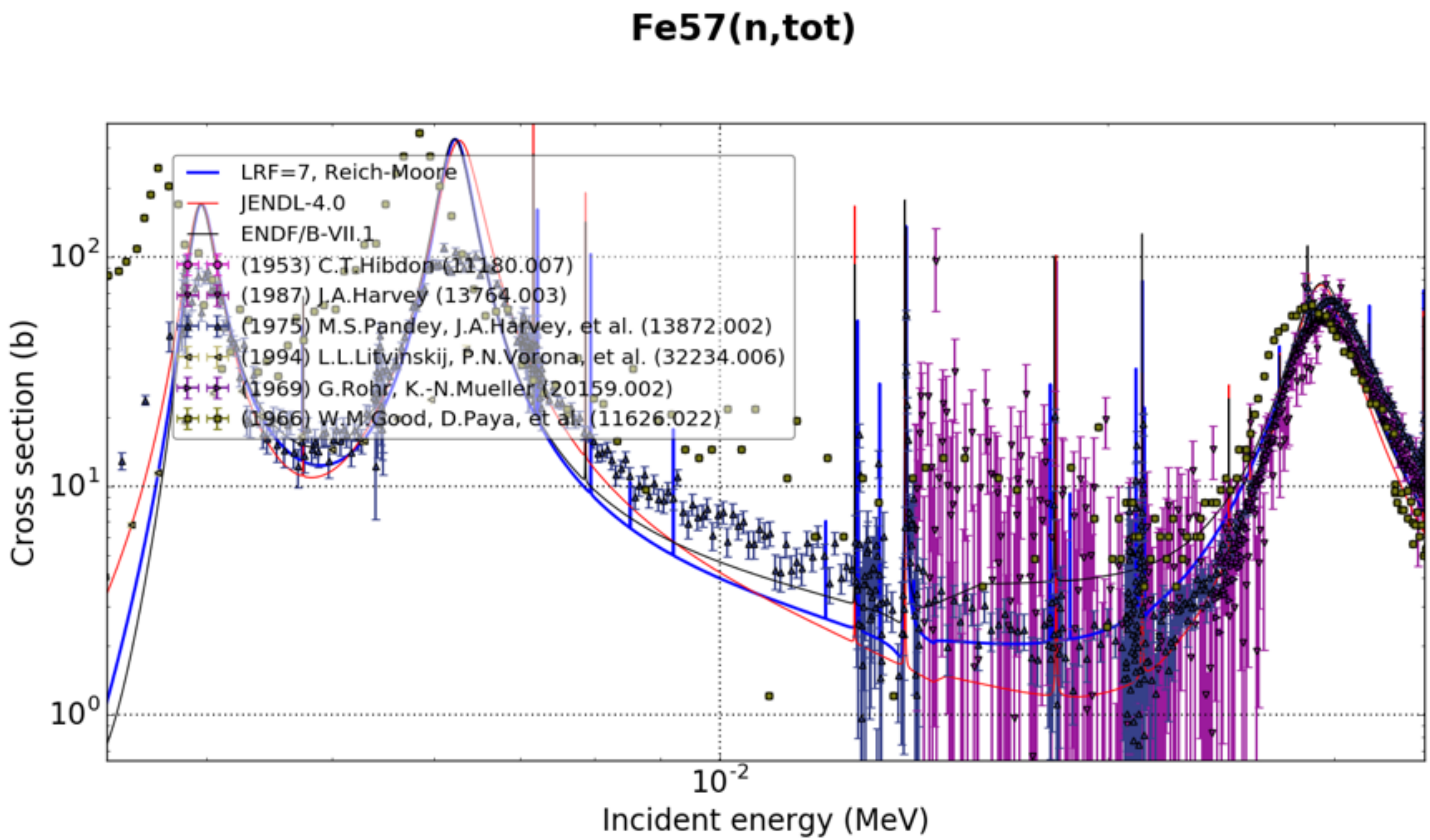


Tweaked bound levels and resonance at 6.22 keV

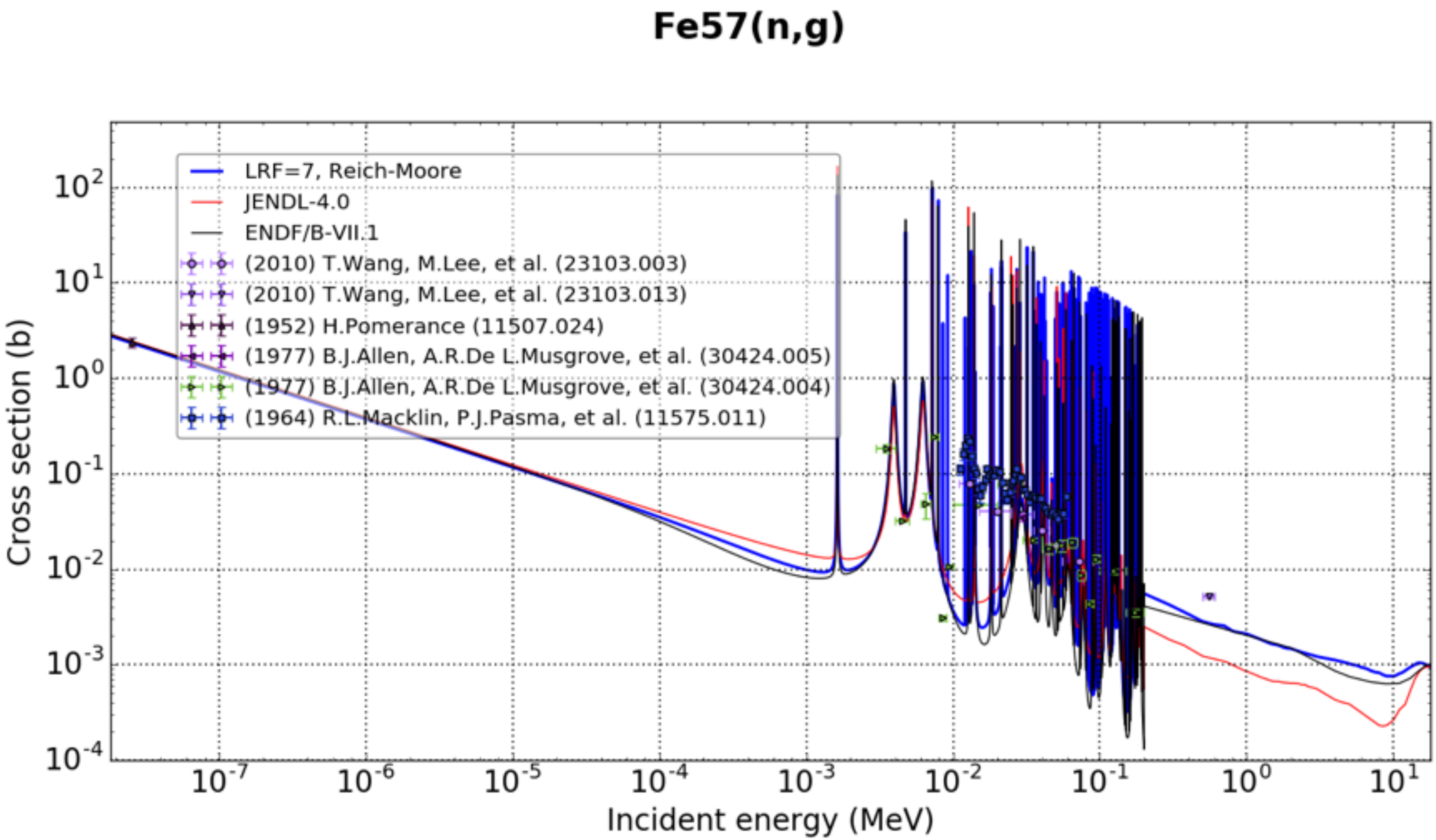
		Before			After		
E_R (kev)	J	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)	Γ_t (eV)	Γ_n (eV)	Γ_γ (eV)
-55.00	0				27,000.8	27,000.0	0.8
-2.33	1	66.62	64.89	1.73			
-1.22	1				11.51	9.51	2.00
6.22	1	381.15	380.00	1.15	401.15	400.00	1.15

Also, remember R' = 6.3 -> 5.9 fm

After: Nail valley



get thermal dead on (by design)



6. Do we still match the MACS(30 keV) value for capture?

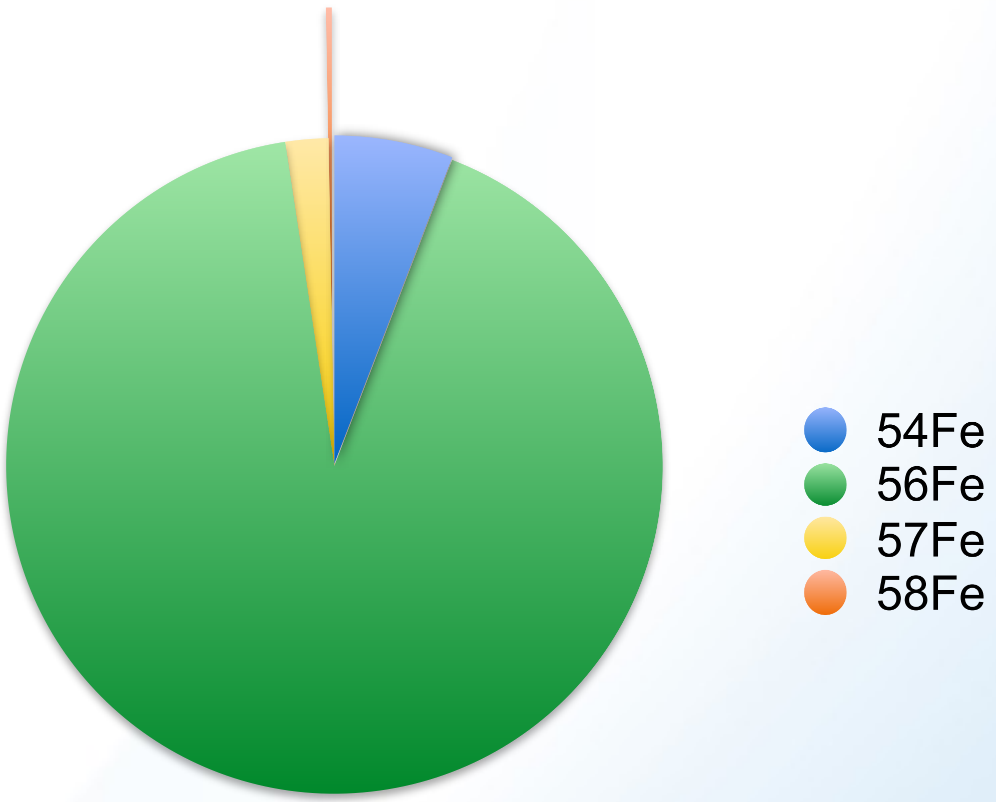
- MACS(30 keV) very useful for quick-n-dirty data validation
- Bao et al. values are the experimental values compiled in Bao et al. At. Data & Nucl. Data Tables **76**, 70-154 (2000)
- Given the spread in experimental data, the LRF=7 values are probably good enough

Source	MACS(30 keV)
MLBW	41.38 mb
LRF=7	36.02 mb
Atlas (exp)	36.0 +/- 2.7 mb
Atlas (calc)	42.1 +/- 8.4 mb
Kadonis-0.3	32 mb
Bao et al. (1)	39.9 +/- 4 mb
Bao et al. (2)	36.0 +/- 2.3 mb
Bao et al. (3)	28 +/- 6 mb

^{58}Fe

Fast

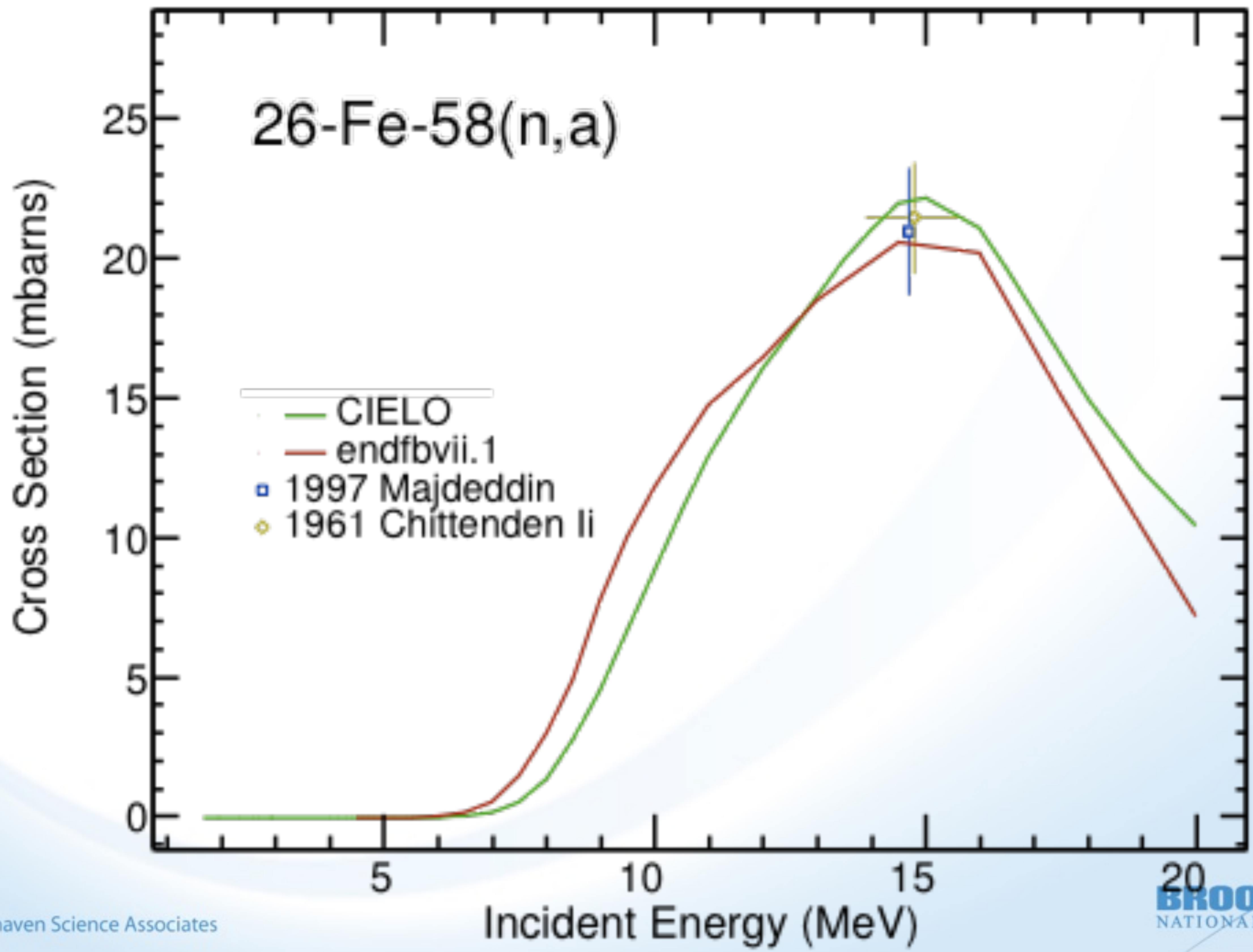
- Soukhovitskii-Capote OMP for even iron isotopes
- No reduction of (n,tot) necessary
- Even fewer experimental datasets (No dosimetry file)
- Fit (n,a) to the few experiments available



Resonances

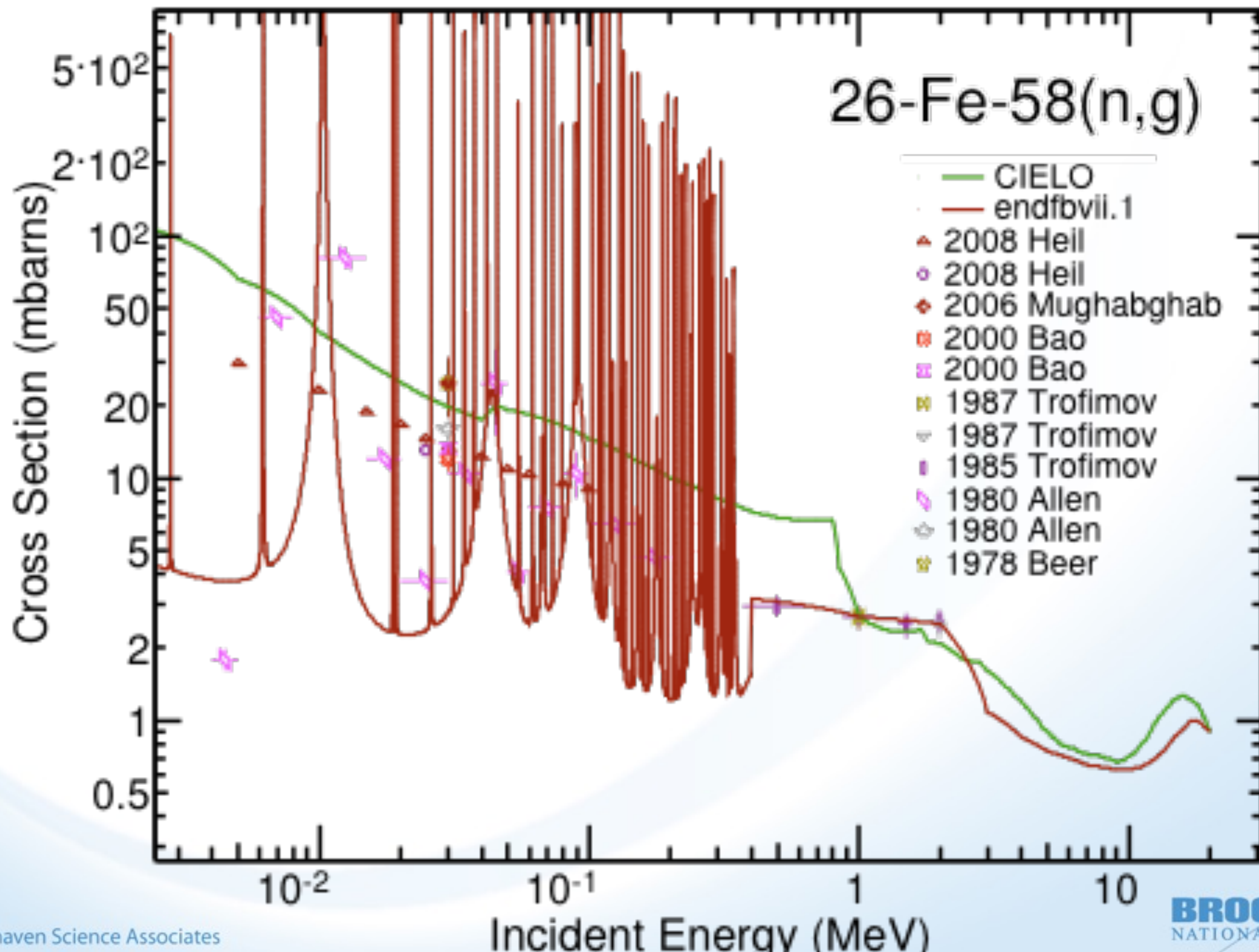
- From Moxon

^{58}Fe



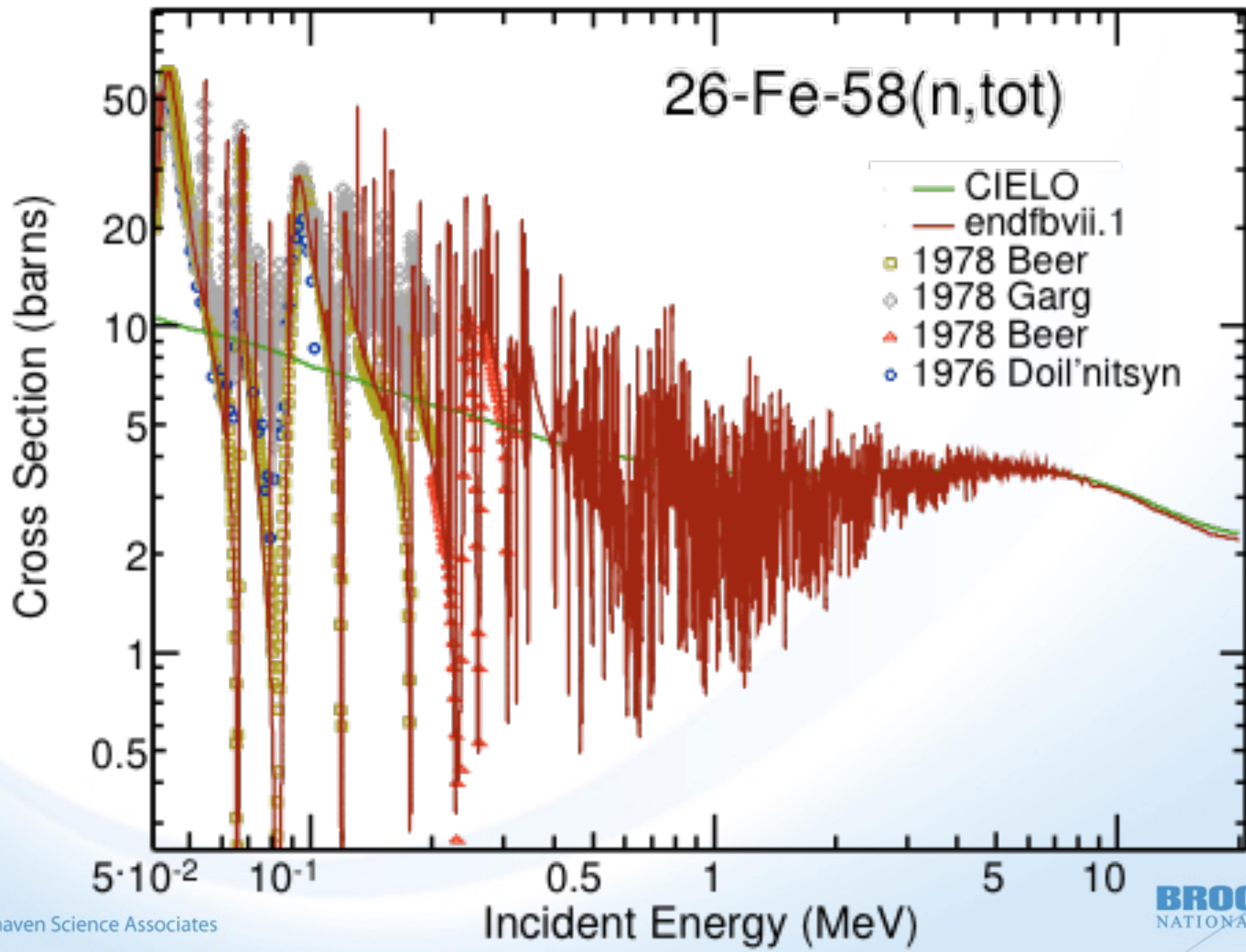
26-Fe-58(n,a)
Cross Section (mbarns)
Incident Energy (MeV)
CIELO
endfbvii.1
1997 Majdeddin
1961 Chittenden Ii
0
5
10
15
20
25
5
10
15
20

^{58}Fe



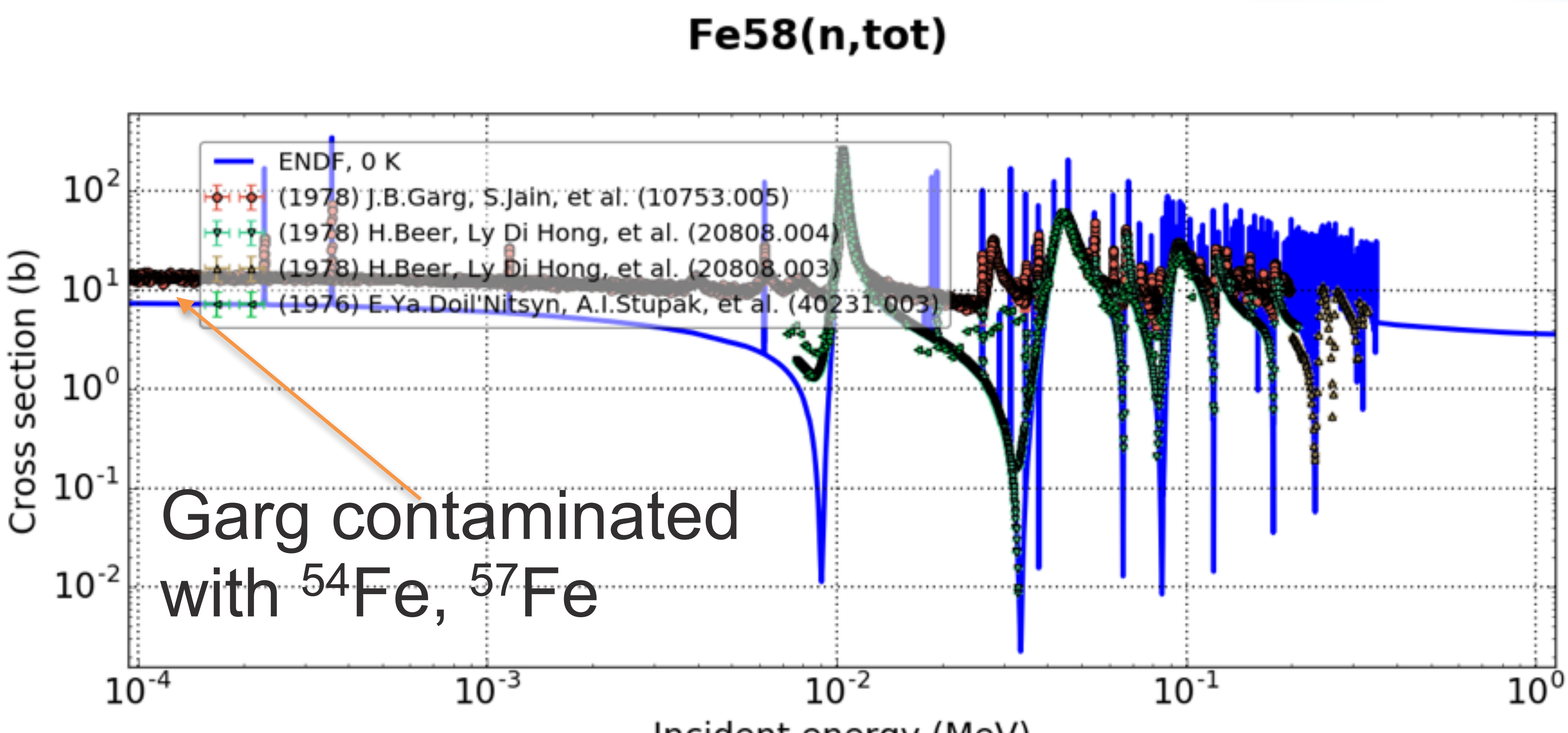
26-Fe-58(n,g)
CIELO
endfbvii.1
2008 Heil
2008 Heil
2006 Mughabghab
2000 Bao
2000 Bao
1987 Trofimov
1987 Trofimov
1985 Trofimov
1980 Allen
1980 Allen
1978 Beer
Cross Section (mbarns)
5·10²
2·10²
10²
50
20
10
5
2
1
0.5
10⁻²
10⁻¹
1
10
Incident Energy (MeV)

^{58}Fe


26-Fe-58(n,tot)
CIELO
endfbvii.1
1978 Beer
1978 Garg
1978 Beer
1976 Doil'nitsyn
Cross Section (barns)
50
20
10
5
2
1
0.5
5·10-2
10-1
0.5
1
5
10
Incident Energy (MeV)

^{58}Fe: from Moxon

Moxon evaluation taken from JEFF-3.2. The unresolved region is for self-shielding only. All angular distributions, including RRR and URR, are calculated by EMPIRE.



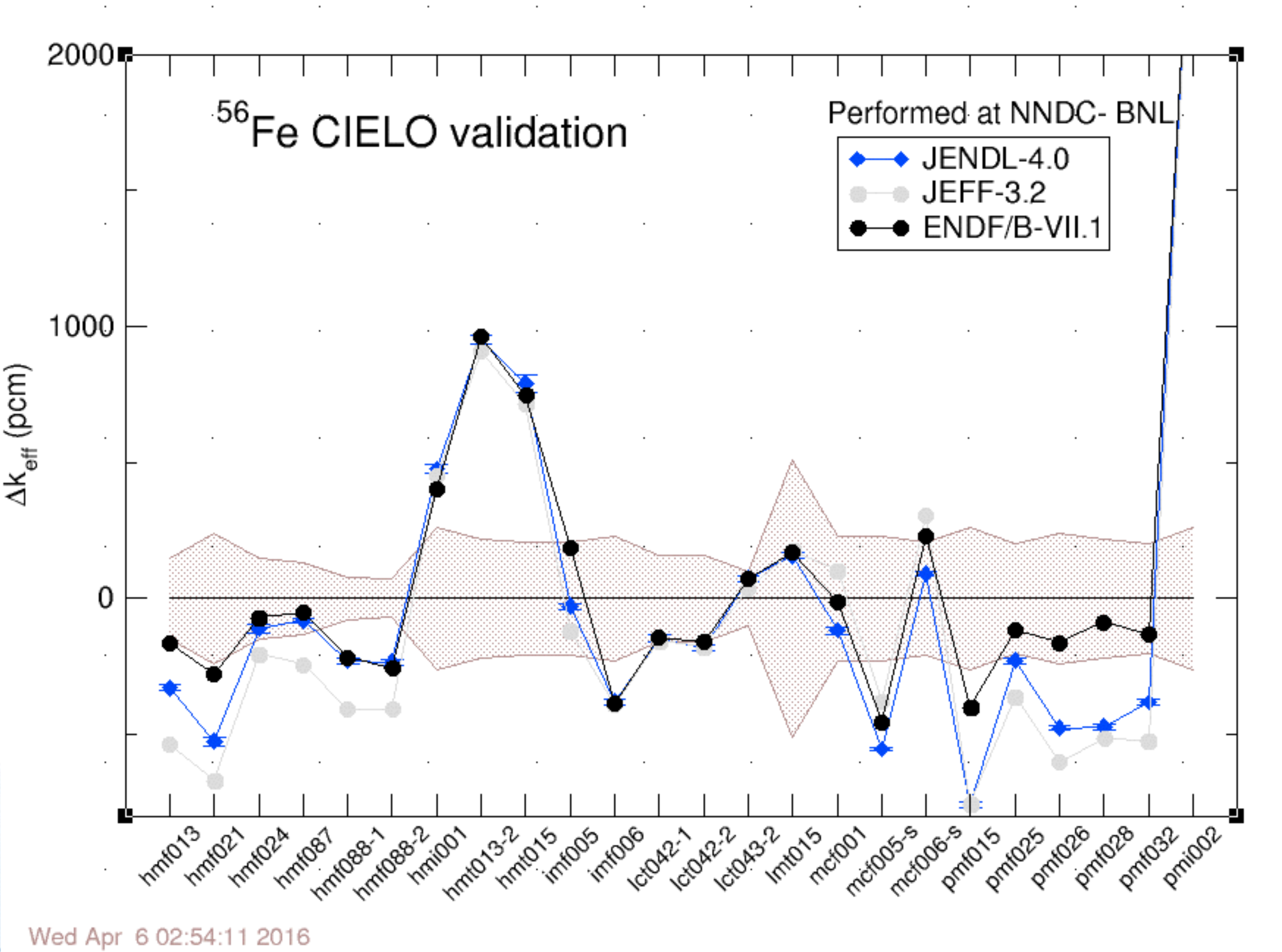
ICSBEP Validation at the NNDC

- CIELO 54Fe rev.222
- CIELO 56Fe rev.219
- CIELO 57Fe rev.234
- CIELO 58Fe rev.224
- ENDF/B-VII.1 (official LANL ACE lib.)

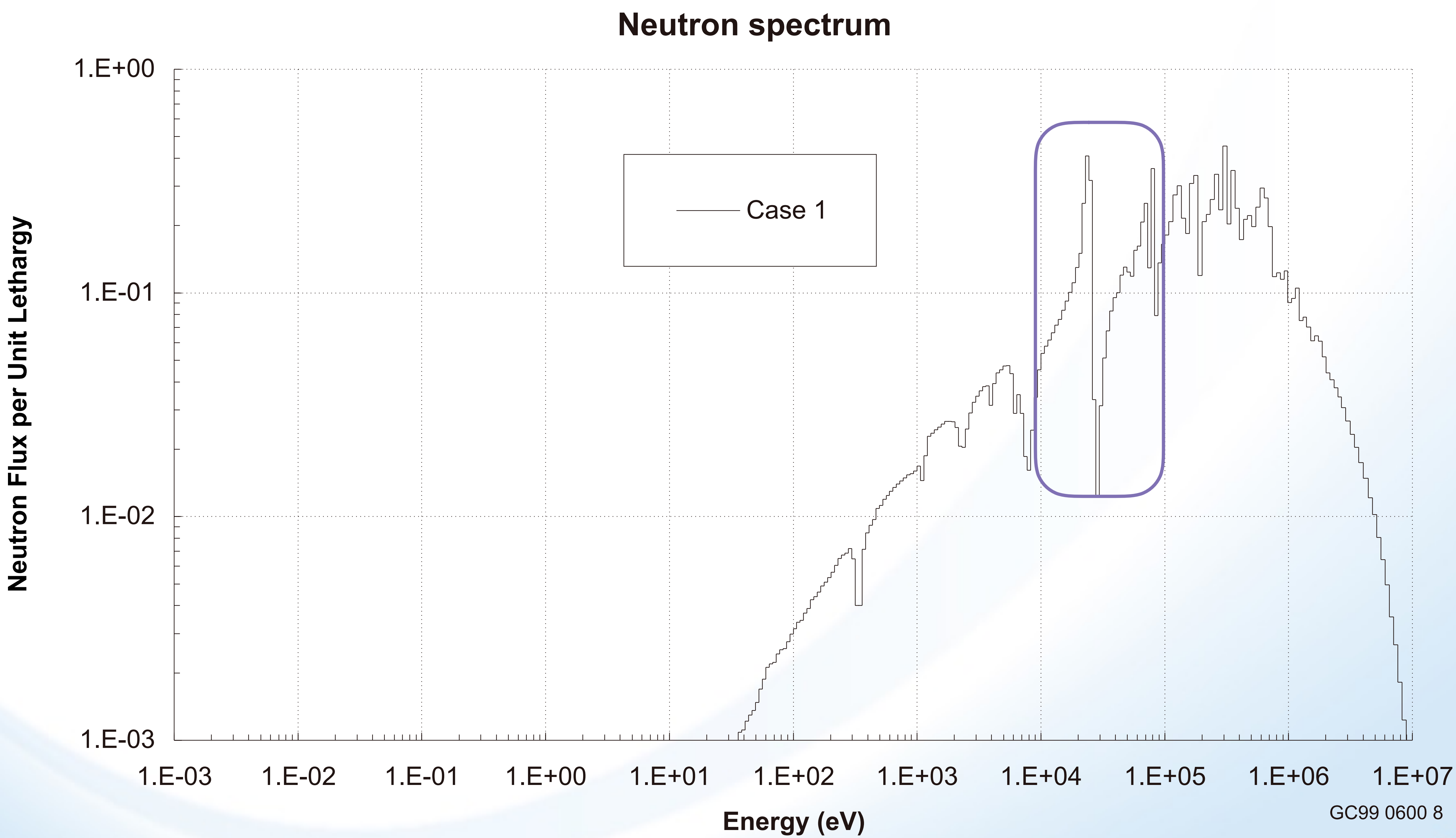
On what do we test?

	ICSBEP name	Common name
1	PU-MET-FAST-015	BR-1-3
2	PU-MET-FAST-025	pmf025
3	PU-MET-FAST-026	pmf026
4	PU-MET-FAST-028	pmf028
5	PU-MET-FAST-032	pmf032
6	HEU-MET-FAST-013	VNIITF-CTF-SS-13
7	HEU-MET-FAST-021	VNIITF-CTF-SS-21
8	HEU-MET-FAST-024	VNIITF-CTF-SS-24
9	IEU-MET-FAST-005	VNIITF-CTF-SS-5
10	IEU-MET-FAST-006	VNIITF-CTF-SS-6
11	HEU-MET-FAST-087	VNIITF-CTF-Fe
12	HEU-MET-FAST-088	hmf088-1
13	HEU-MET-FAST-088	hmf088-2
14	LEU-COMP-THERM-042	lct042-1
15	LEU-COMP-THERM-042	lct042-2
16	LEU-COMP-THERM-043	IPEN/MB-01
17	LEU-MET-THERM-015	lmt015
18	HEU-MET-THERM-013	hmt013-2
19	HEU-MET-THERM-015	hmt015
20	HEU-MET-INTER-001	ZPR-9/34
21	PU-MET-INTER-002	ZPR-6/10
22	MIX-COMP-FAST-001	ZPR-6/7
23	MIX-COMP-FAST-005	ZPR-9/31
24	MIX-COMP-FAST-006	ZPPR-2

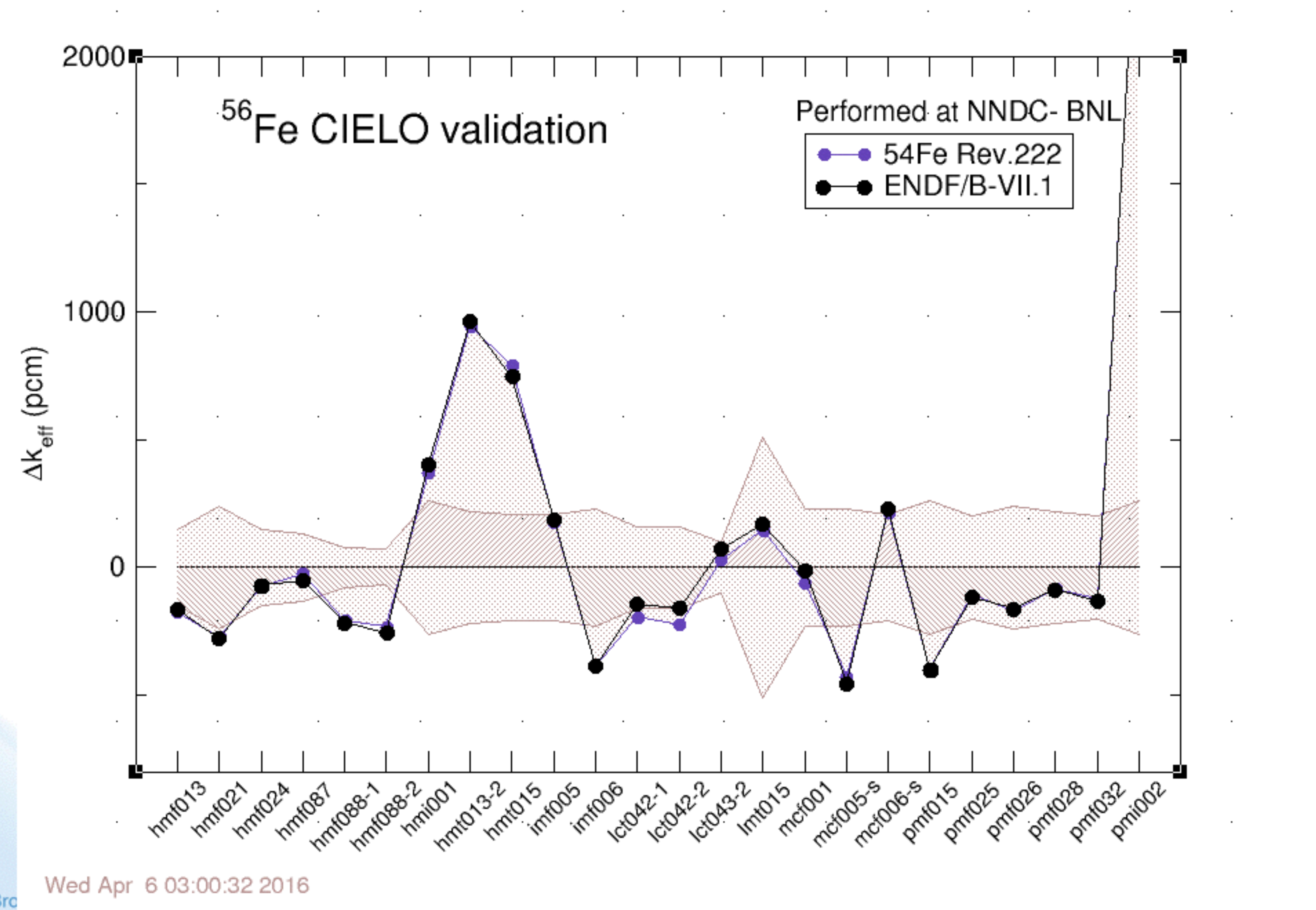
Starting point VII.1 v. JENDL-4.0 v. JEFF-3.2



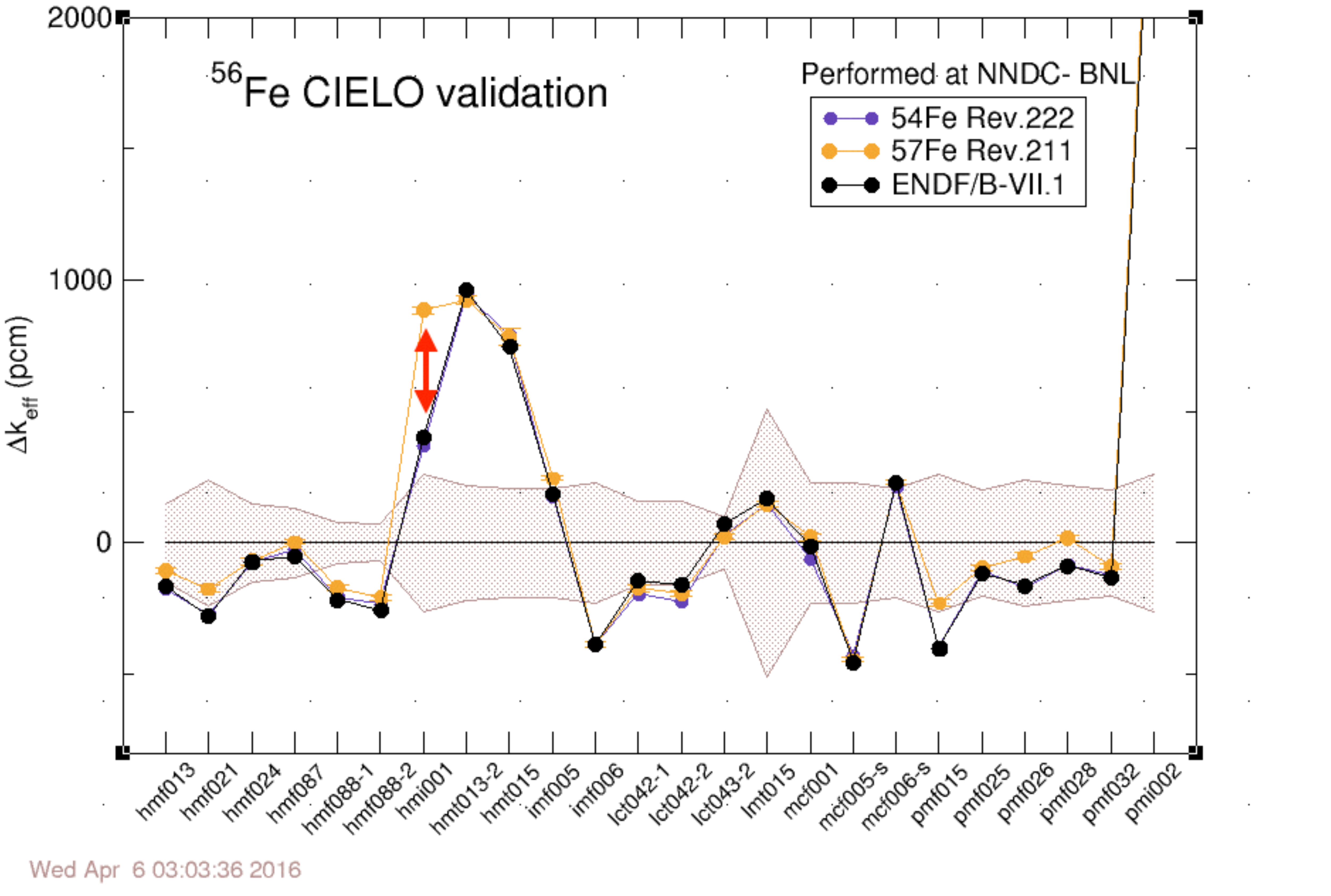
HEU-MET-INTER-001 very sensitive to 10 - 50 keV part of cross section



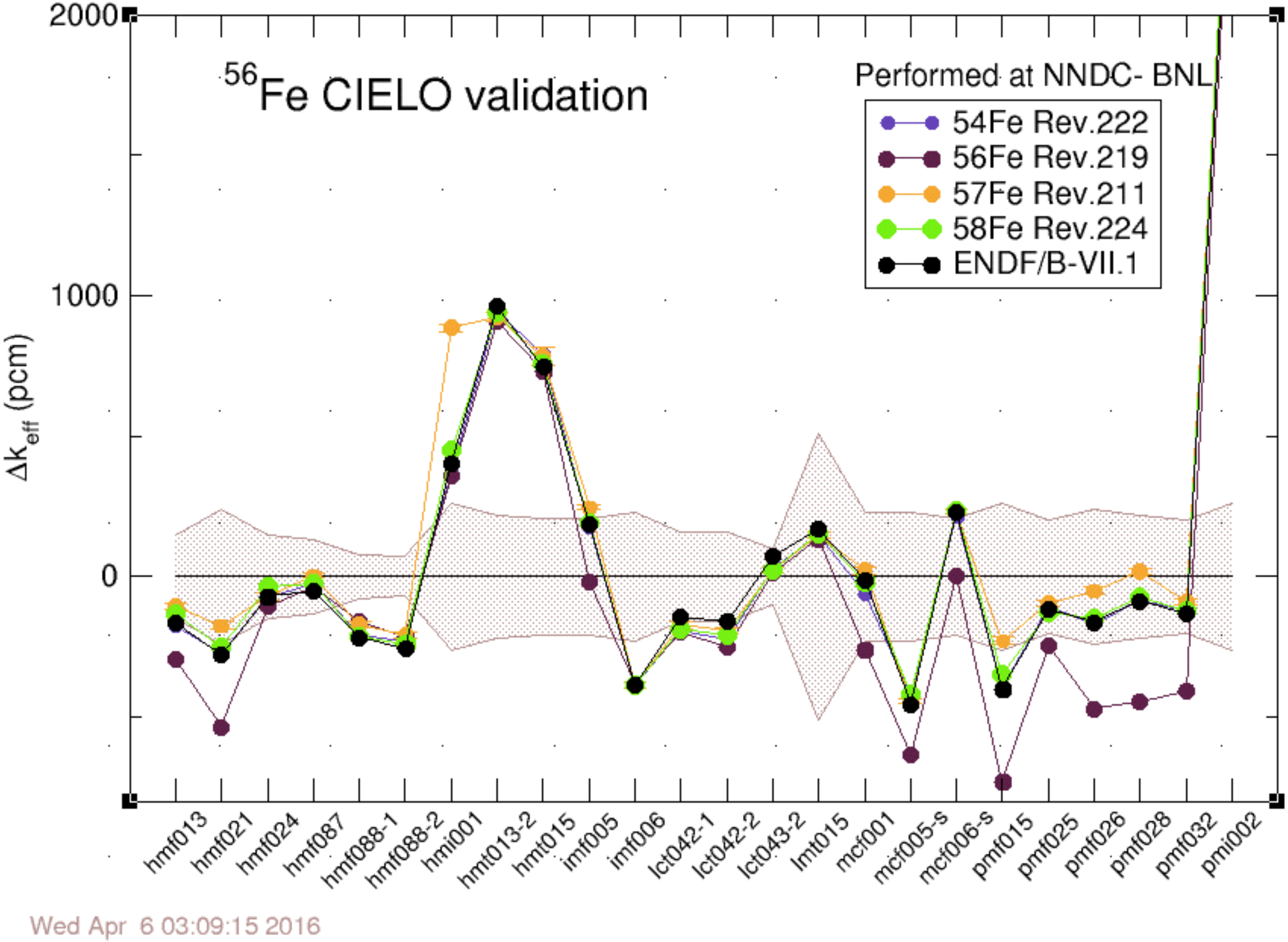
ENDF/B-VII.1 + CIELO 54Fe



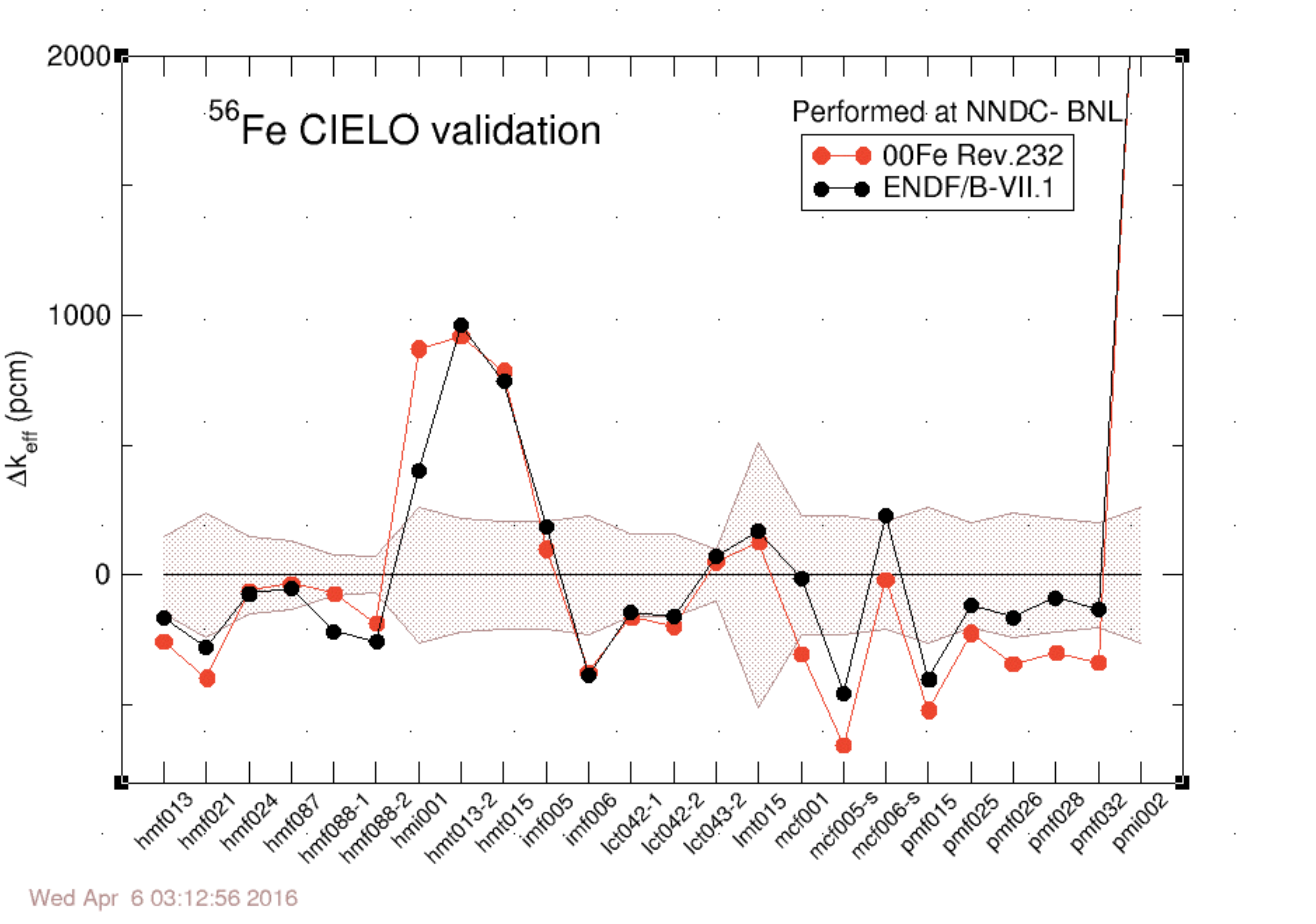
…adding CIELO 57Fe



…adding CIELO 56Fe and 58Fe



ENDF/B-VII.1 + CIELO natFe



Conclusions

- First versions of evaluated files for iron isotopes are ready
- Promising results even though minor improvements will be necessary
- Preliminary calculations of covariances were performed for main reactions
- Validation and tests have begun
- Consistency among isotope parameters
- To our knowledge, first ever non-SAMMY LRF=7 resonance evaluation

MACS (30 keV)

	β0	KADONIS	ENDF/B-VII.1*	JENDL-4.0*
^{54}Fe	28.3±1.3	29.6±1.3	21.6±2.7	21.6
^{56}Fe	11.2±1.1	11.7±0.5	11.5±1.1	11.8
^{57}Fe	36.02	40.0±4.0	28.5±4.6	30.2
^{58}Fe	13.7±1.5	13.5±0.7	19.7	14.0

**B. Pritychenko and S. F. Mughabghab, Nuclear Data Sheets 113, 3120 (2012)*