CIELO Progress on 56Fe

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U.S. DEPARTMENT OF ENERGY | Office of Science

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CIELO-Iron collaboration

BNL, CNDC, IAEA, IRM, JSI, LANL, ORNL, RPI, IRSN

- Exp. data analysis: CNDC
- Resonance range: ORNL & IRSN & BNL & IAEA
- Fast neutron range: EMPIRE (BNL, IAEA)
- File assembly: IAEA, BNL
- Testing: IAEA, RPI, BNL, LANL, JSI

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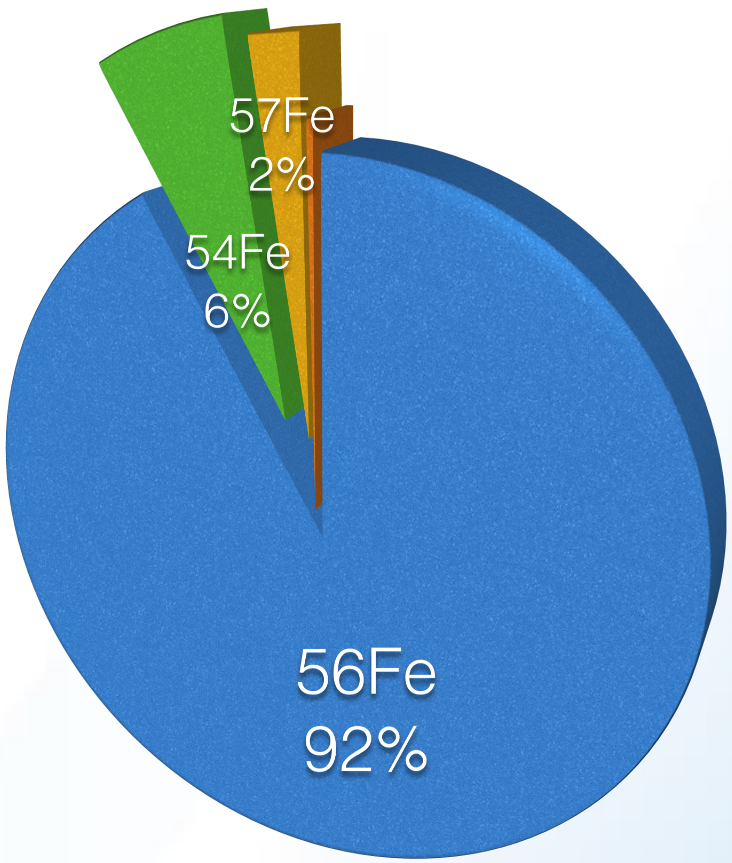
1. BNL, Upton, NY, USA
2. IAEA, Vienna, Austria
3. ORNL, Oak Ridge, TN, USA
4. EC-JRC-IRMM, Geel, Belgium
5. RPI, Troy, NY, USA
6. CNDC, Beijing, P.R.China
7. CIAE, Beijing, P.R.China
8. IRSN, Paris, France
9. ITA, Sao José dos Campos, Brazil
10. Bucharest University, Bucharest-Magurele, Romania

Features of CIELO Iron evaluation

- Strong reliance on experimental data including recent Geel, LANL and RPI
- IRDFF data adopted whenever available
- Model calculations adjusted to reproduce IRDFF and exp. data
- Special attention devoted to angular distributions (AD)
  - AD derived from resonance parameters
  - anisotropic AD compound nucleus inelastic scattering
  - influence of AD on benchmark results



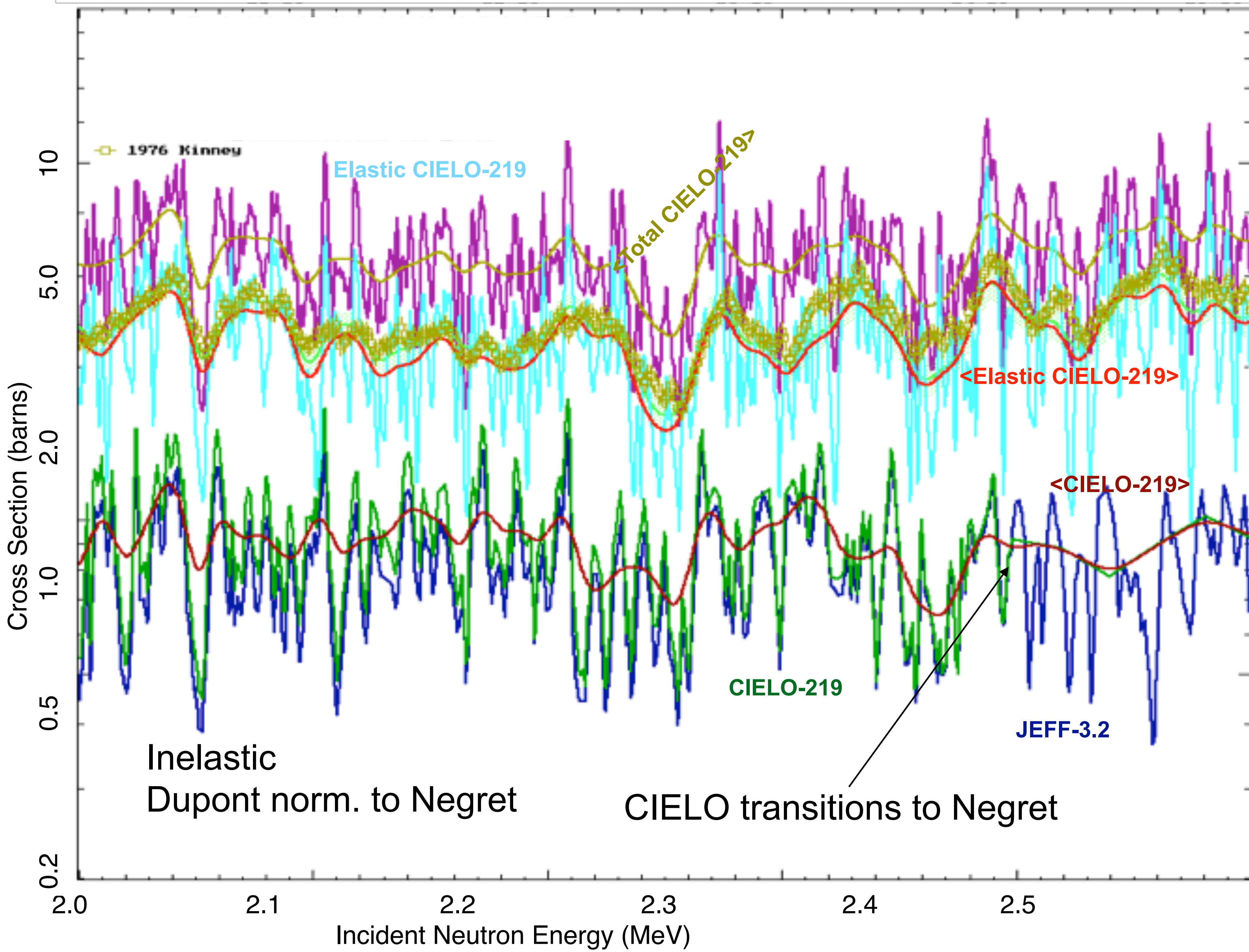
- All reaction channels up to (n,xn) and (n,xp) treated as exclusive and continued smoothly to 150 MeV
- Simultaneous evaluation of minor isotopes ^{54}Fe, ^{57}Fe and ^{58}Fe

Summary of ^{56}Fe releases

^{56}Fe	RRR	Fast
β-1	• **JENDL-4.0** up to 850 keV • Artificial “background" added to capture around 20 keV • Background near 800 keV was reduced by 50% • Elas. ang. dist. from JENDL-4.0 • Tweak of P2 and P4 Legendre coefficients of elastic above 0.3 MeV • Res. @ 766.7 keV was corrected	• Gilbert-Cameron level-densities • Total taken from JEFF-3.2 • Ang. dist. up to 4MeV taken from JEFF-3.2 • Tweak of P2 and P4 Legendre coefficients of elastic below 1.5 MeV
β-2	• Revised resonance region from **IRSN** up to 850 keV in the LRF=7 format • No P2, P4 tweaks • Elastic angular distributions reconstructed from resonance parameters - IRSN < 850 keV	• Elastic and inelastic cross sections and angular distributions taken from beta 1 • Switch from pure GDR strength function to **Weisskopf** improving agreement of inelastic with experiment.
β-3	• **Back to Beta-1** including P2, P4 tweaks • Elas. ang. dist. taken from resonance parameters of JENDL-4.0 < 850 keV	• Capture above 860keV adjusted to **RPI data** • Higher energies: EMPIRE as in β-2 • **Experimental inelastic and elastic** <4 MeV • Improved alpha production • **HMS** above 30 MeV

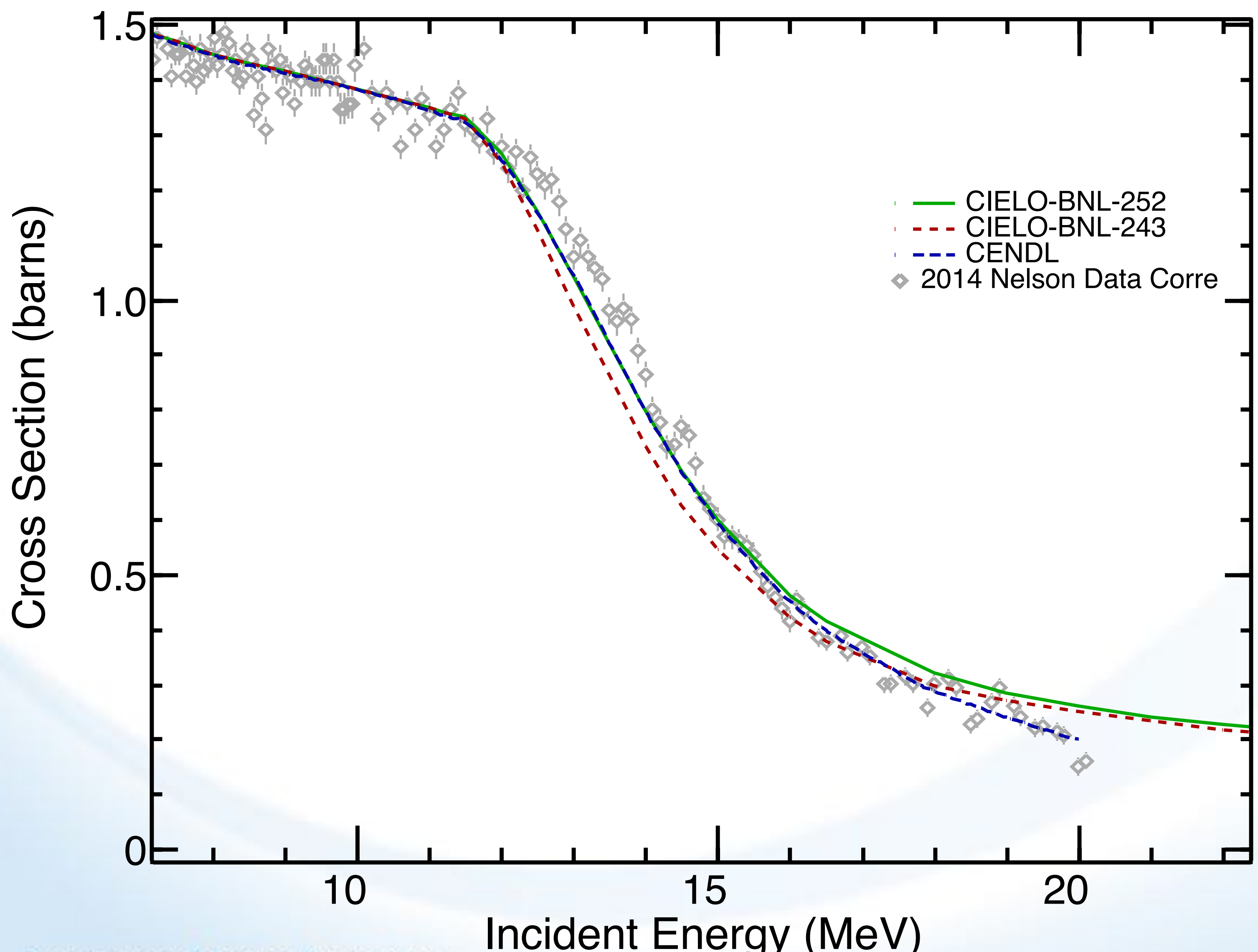
Consistent usage of exp. data:

(i) total from Berthold (corrected for minor isotopes)
(ii) inelastic - Dupont normalized to Negret up to 2.4 MeV, Negret above,
(iii) elastic = total - inelastic. Resolution broadened elastic agrees with Kinney data.



Rising inelastic shoulder - ^{56}Fe

Compared to CENDL and VII.1 our CIELO rev.243 inelastic was too low between 12 and 16 MeV. How to bring it up without destroying perfect agreement for (n,p)?



Solution:
Increase competition of gammas against neutron emission from ^{56}Fe by increasing gamma-ray strength function in ^{56}Fe.

Inelastic goes up, (n,2n) goes down (we like it), (n,p) remains untouched and gamma spectra calculate closer to the experiment.

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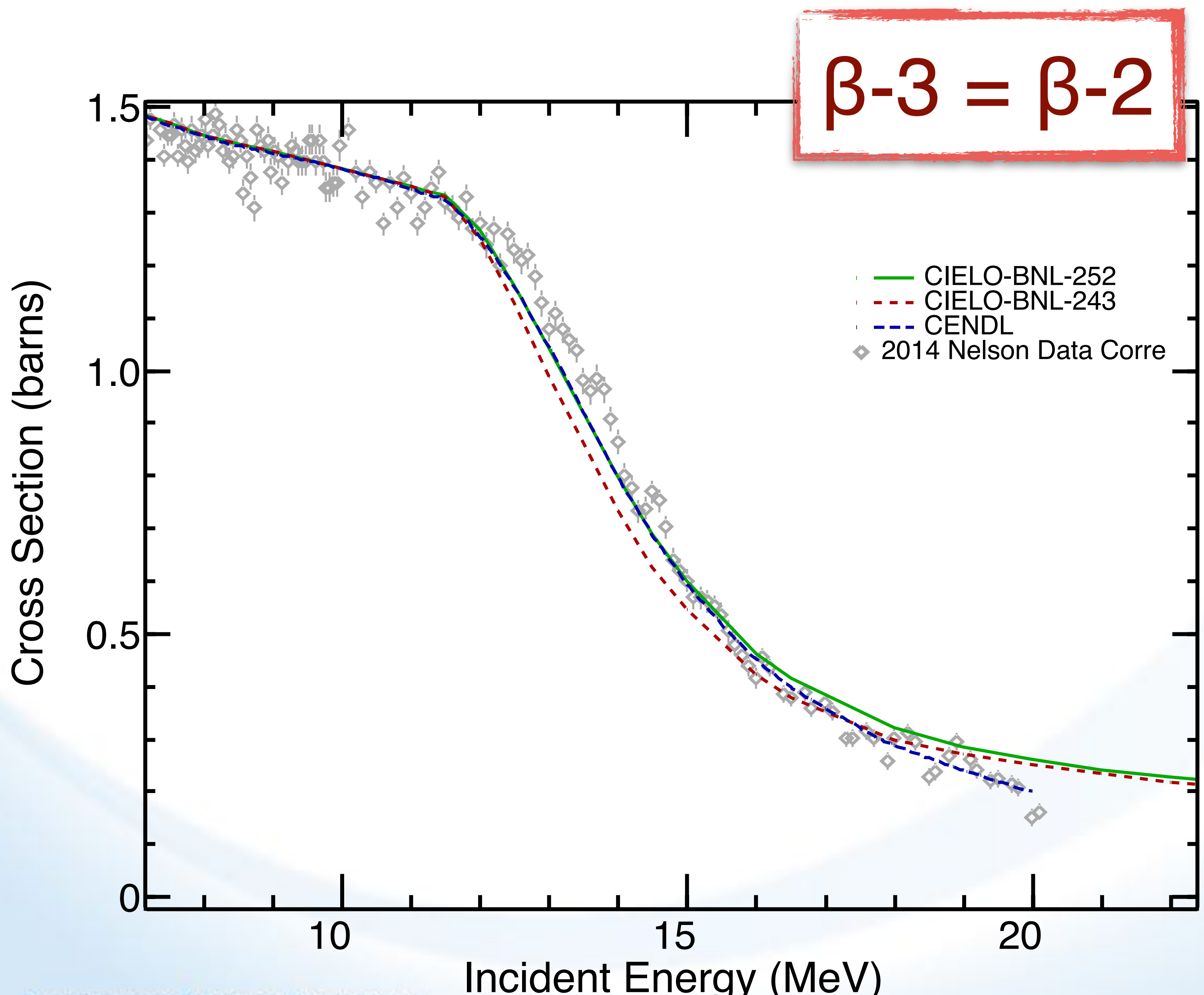

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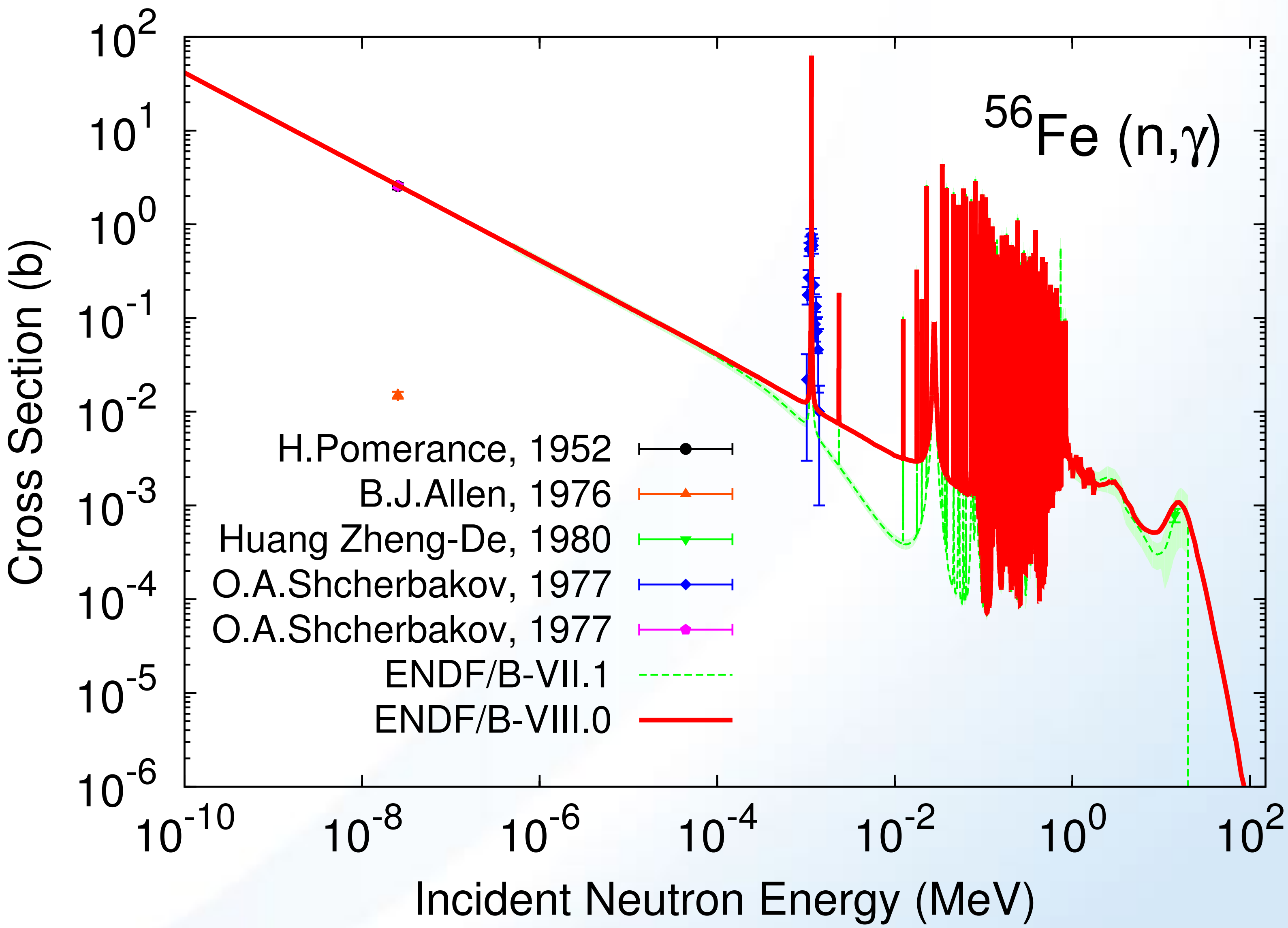
Summary of ^{56}Fe releases (cont.)

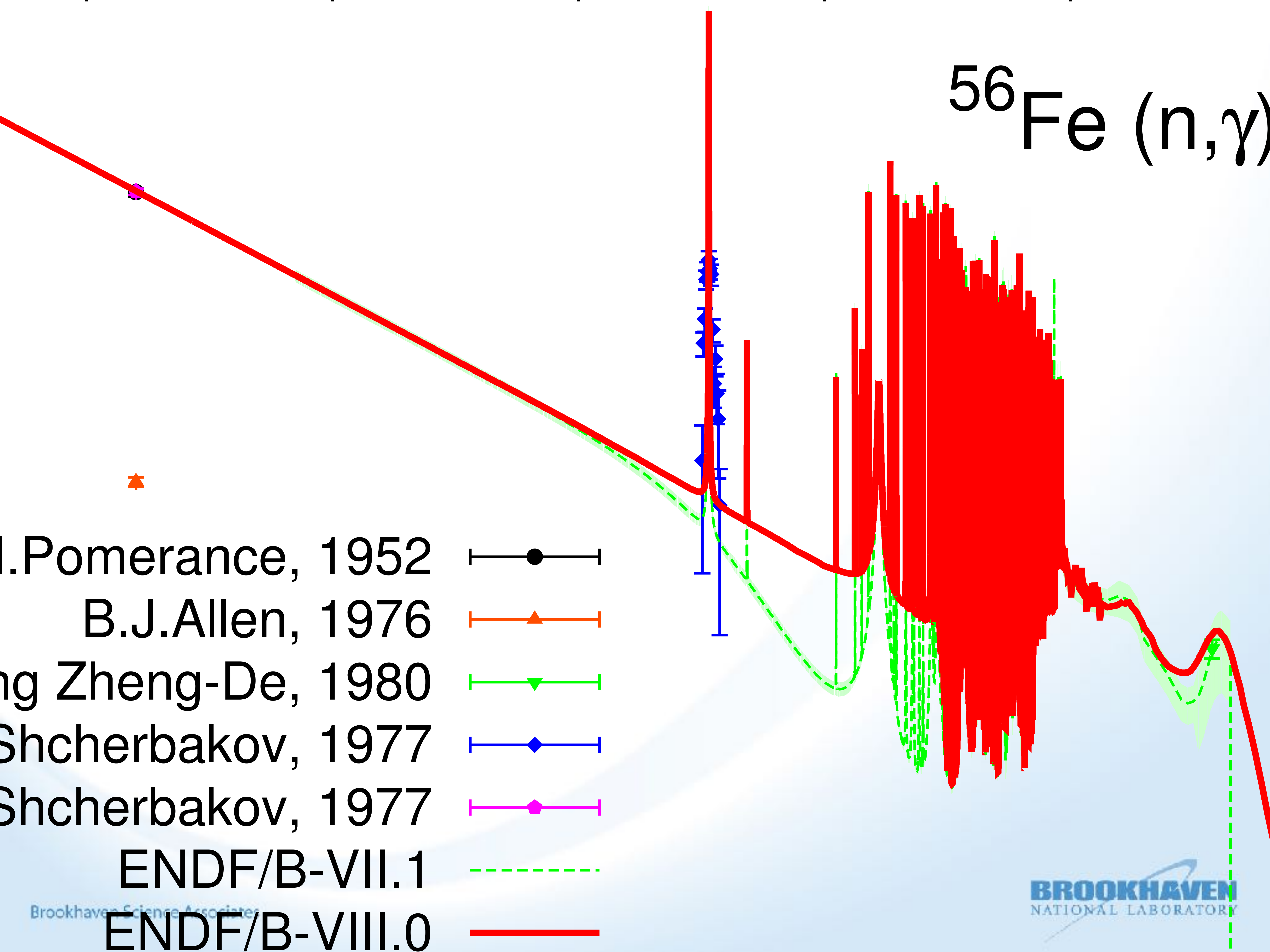
^{56}**Fe**	**RRR**	**Fast**
β-4	• Beta-3 maintained • Capture background around 25 keV slightly reduced • Elastic angular distributions **refitted** to Perrey and modified Kinney (β3 tweaks to P2,4 removed)	• **Improve α-spectra** at high-energies (50 - 150 MeV) • Fixed missing **inelastic branching ratios** • Return to **PCROSS** above 20 MeV • **Exclusive spectra** up to 150 MeV for (n,xn) and (n,xp) reactions •

Changes in ^{56}Fe evaluation (β3 => β4)

Capture background around 25 keV slightly reduced

- Originally introduced to improve notoriously bad performance on ZPR-34/9 (hmi01)



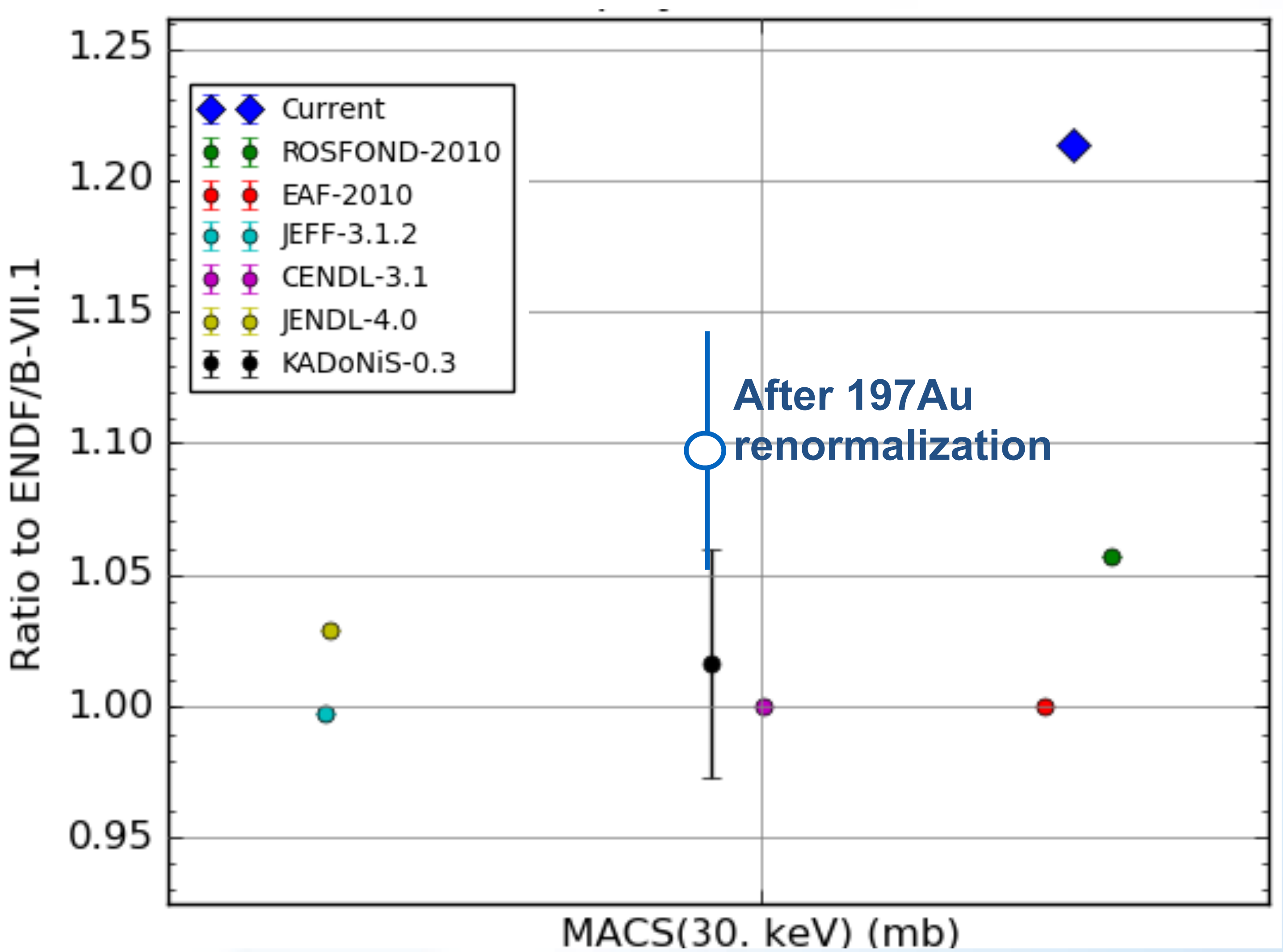


^{56}Fe (n,γ)
Pomerance, 1952
B.J.Allen, 1976
ng Zheng-De, 1980
Shcherbakov, 1977
Shcherbakov, 1977
ENDF/B-VII.1
ENDF/B-VIII.0

Changes in ^{56}Fe evaluation (β3 => β4)

Capture background around 25 keV slightly reduced

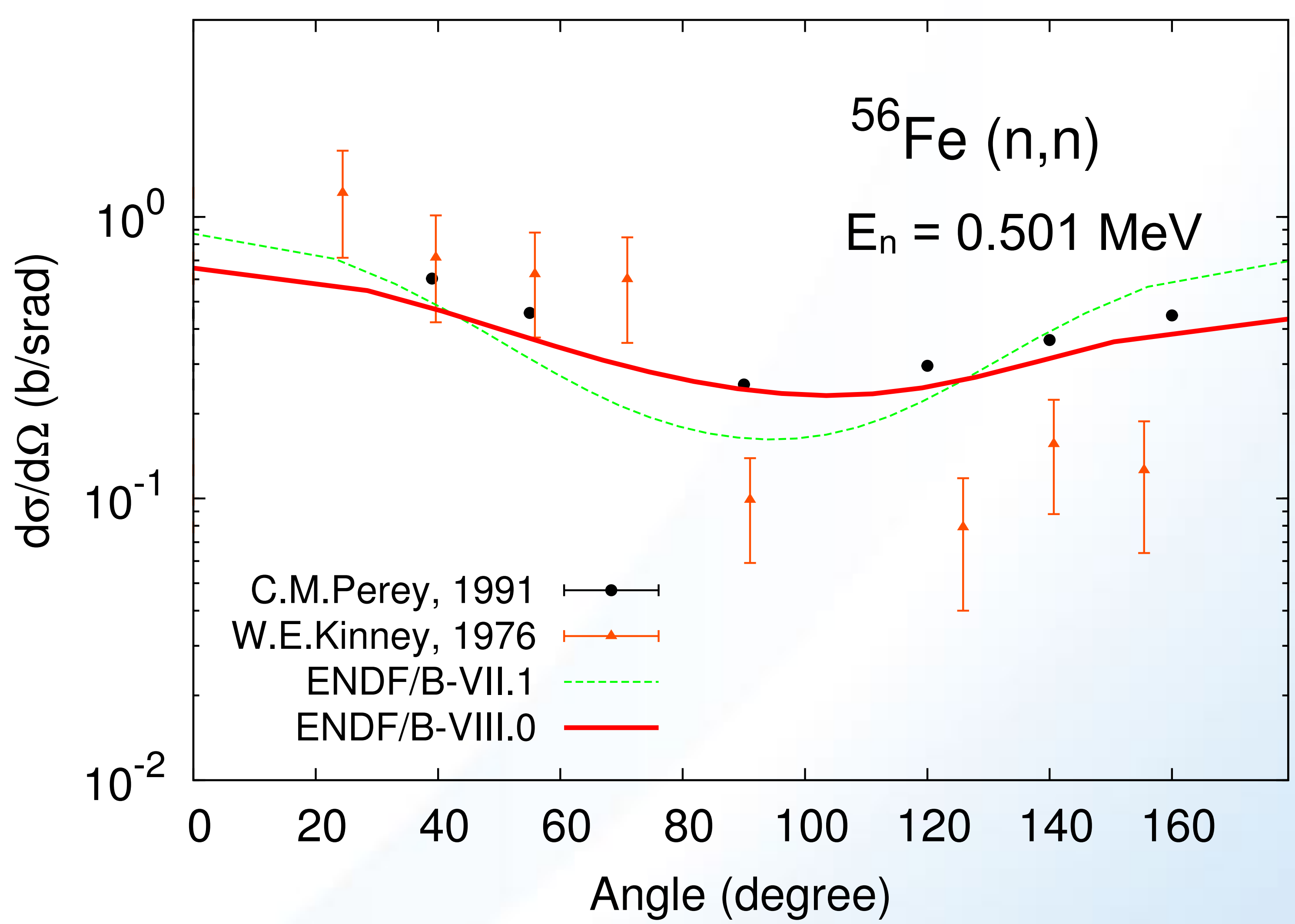
- MACS(@ 30 keV) in mb
  13.97 - VIII.0β4
  11.59 - VII.1
  15.1 +/- 1.3 Mughabghab 06
  11.7 +/- 0.5 KADoNiS v0.3
  (12.4 +/- 0.5 KADoNiS with right 197Au)
- Experimental data:
  13.9 +/- 0.7 Kappeler 1983
  14.4 +/- 2.0 Allen et al, 1977
  15.1 +/- 1.3 Allen et al, 1976
  12.2 +/- 2.1 Wang et al, 10



Changes in ^{56}Fe evaluation (β3 => β4)

Elastic angular distributions refitted (β3 tweaks to $P_{2,4}$ removed)

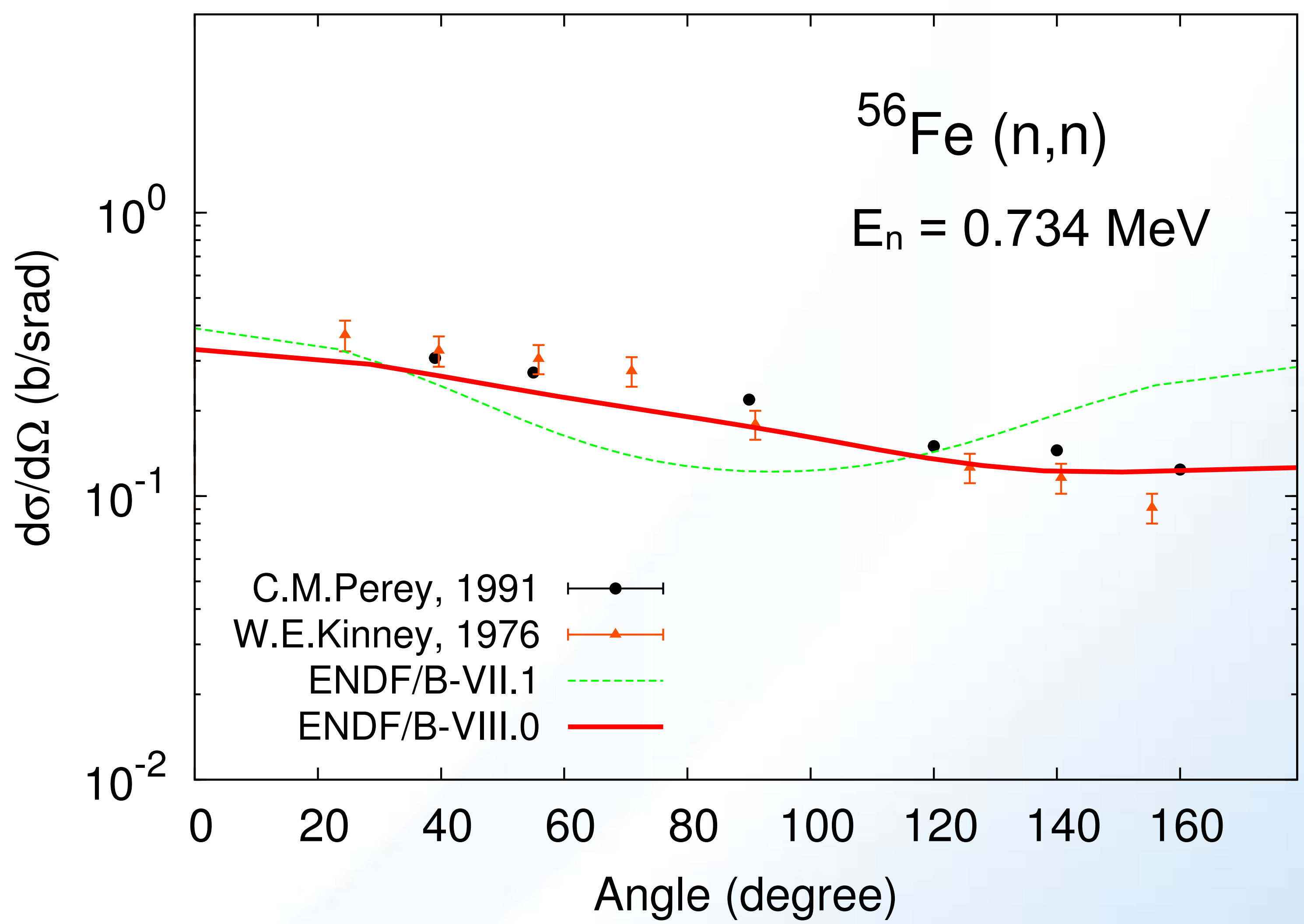
- In the RR range fitted to resolution-broadened Perey data.
- Above the RR up to 2.5 MeV re-fitted to Kinney data with some adjustments based on the comparison with Perey data.
- In the range 2.5-4.0 MeV fitted to Smith (1973).
- Above 4.0 MeV from Empire calculation.



Changes in ^{56}Fe evaluation (β3 => β4)

Elastic angular distributions

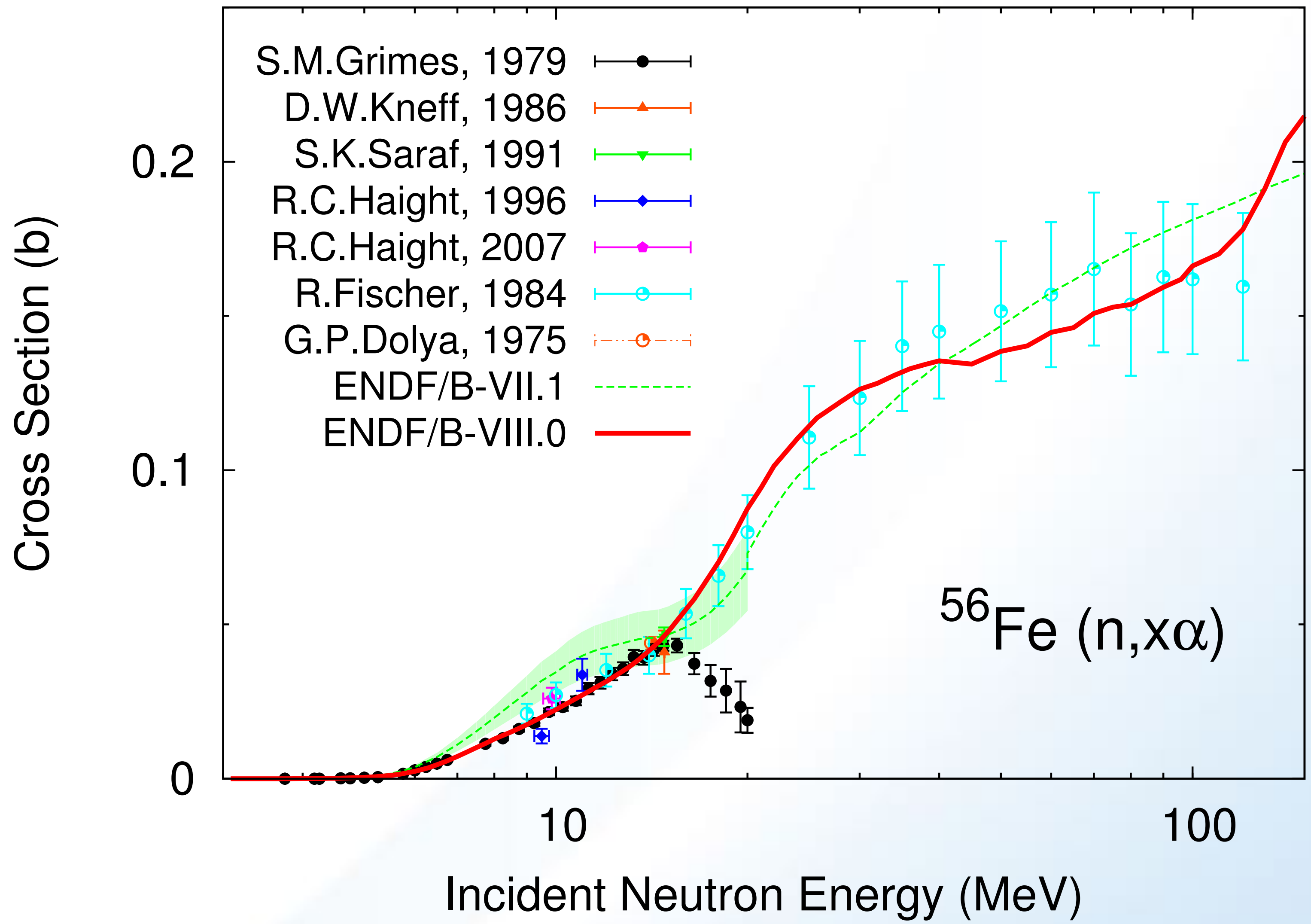
- In the RR range taken from resolution-broadened Perey data.
- Above the RR up to 2.5 MeV re-fitted Kinney data with some adjustments based on the comparison with Perey data in the overlapping region.
- In the range 2.5-4.0 MeV taken from Smith (1973).
- Above 4.0 MeV from Empire calculation.



Changes in ^{56}Fe evaluation (β3 => β4)

Improve α-spectra at high-energies (50 - 150 MeV)

- Identifying which nuclei contribute the most to alpha emissions at 150 MeV and then fitted the level-density and alpha-emission tuning parameters for those nuclei. This fit was done through sensitivity matrix calculations and Kalman.



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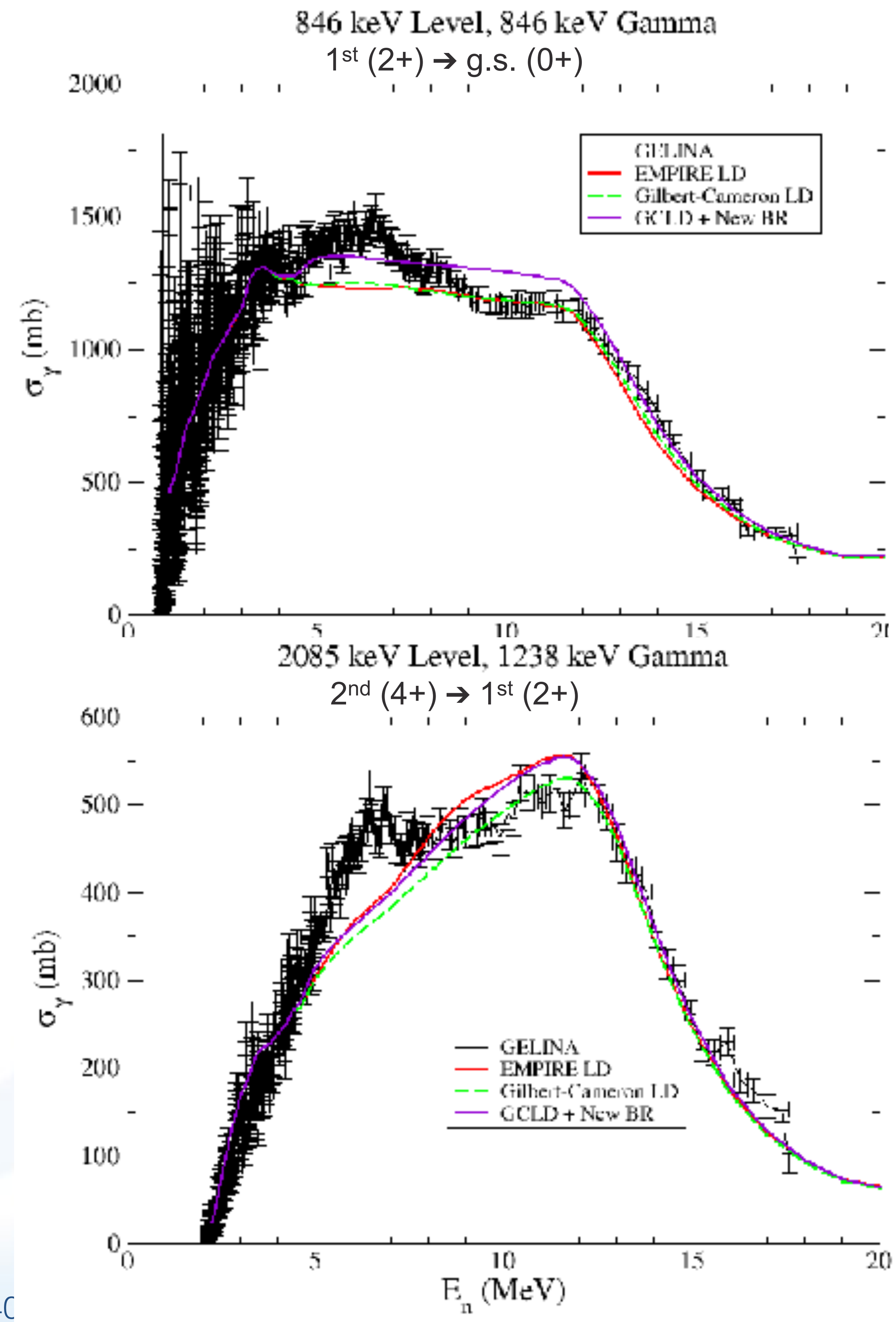
Inelastic γ-rays

Calculations do not get shape right. Possible reasons are:

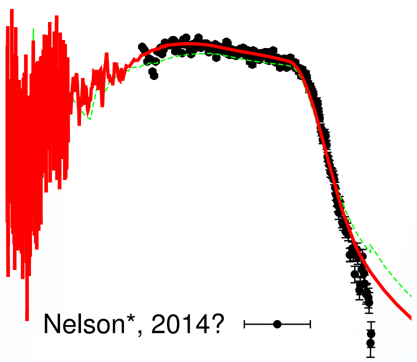
- Too weak direct contribution to the level or/and to the levels above
- Wrong spin or parity of the level (options in ENSDF)
- Missing/wrong branching ratios
- Feeding levels are outside the considered range
- Summation of two or more γ-lines with very close energies

The two plots suggest that feeding from the level(s) above peaking around 6 MeV is missing.

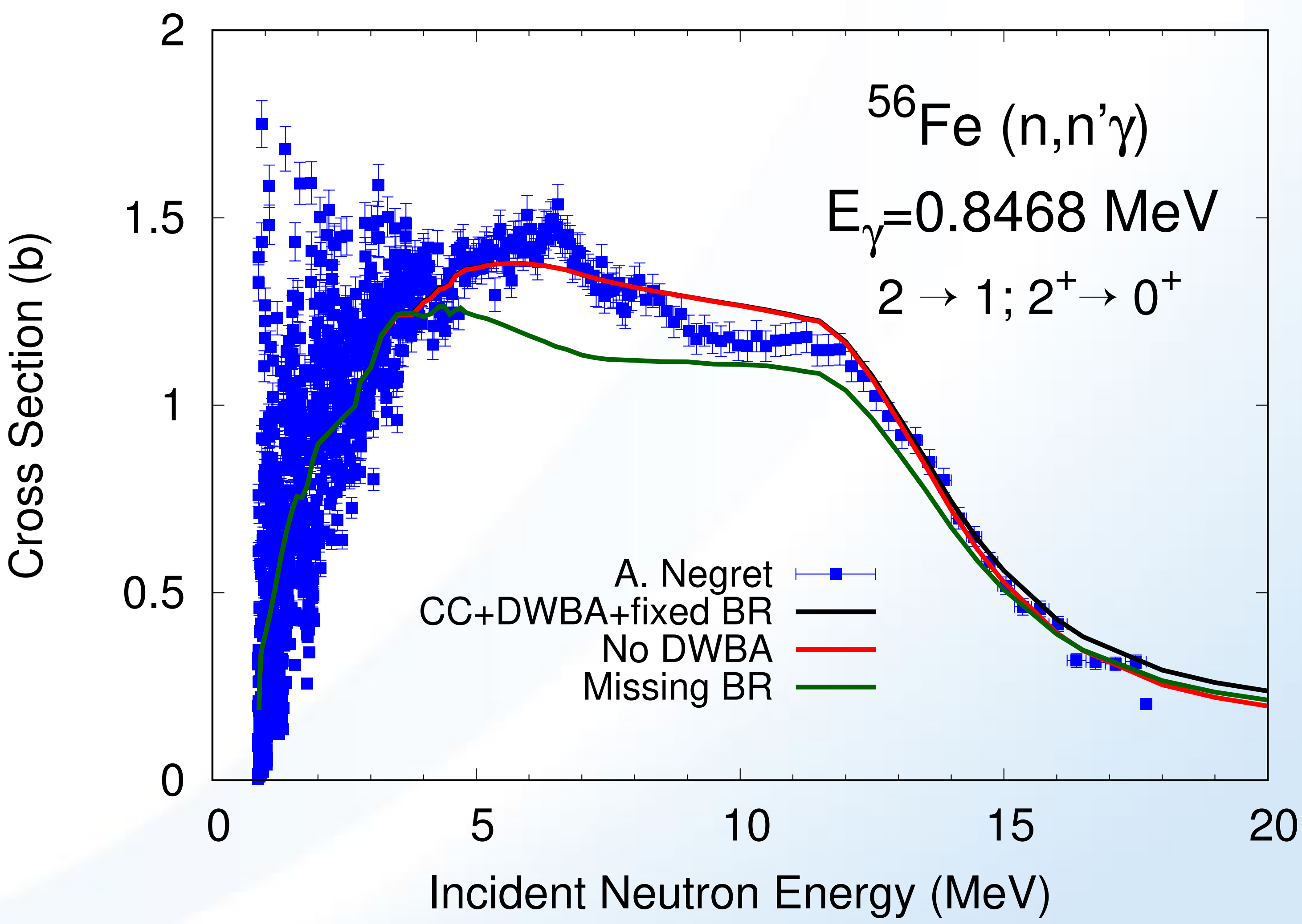


Changes in ^{56}Fe evaluation (β3 => β4)

Complete discrete level decay schemes

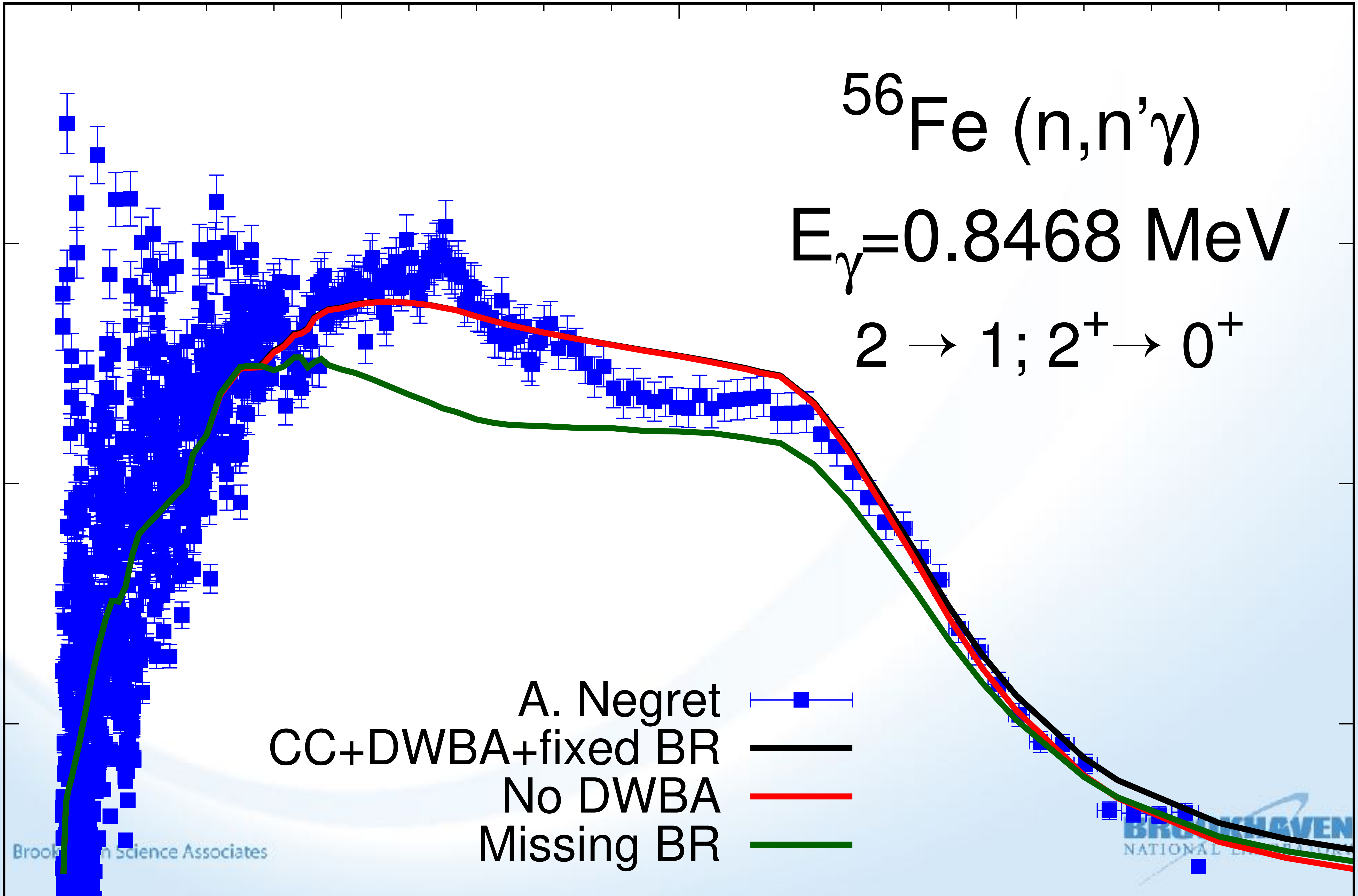


- Fixed missing branching ratios for 56Fe.

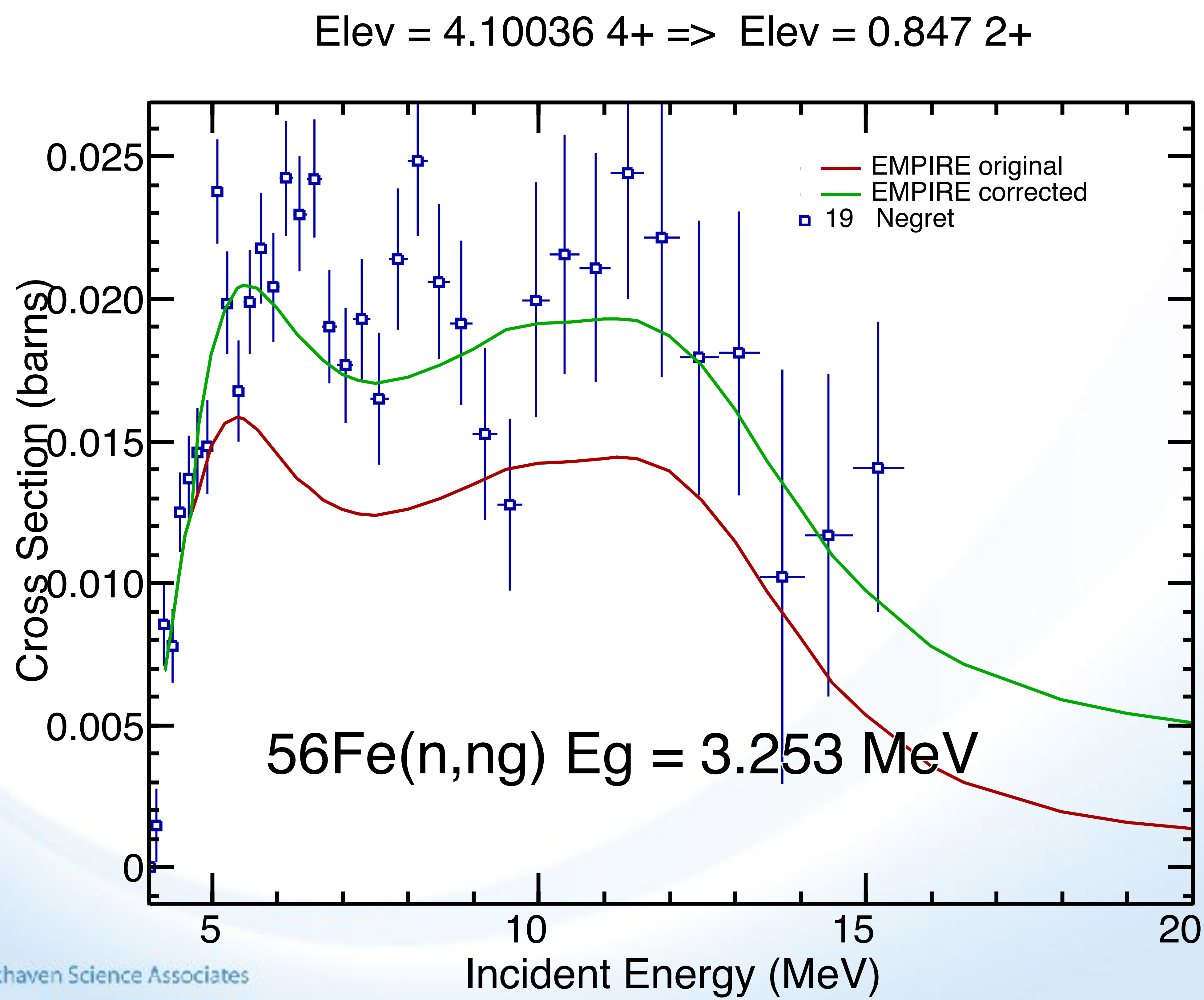


Changes in ^{56}Fe evaluation (β3 => β4)

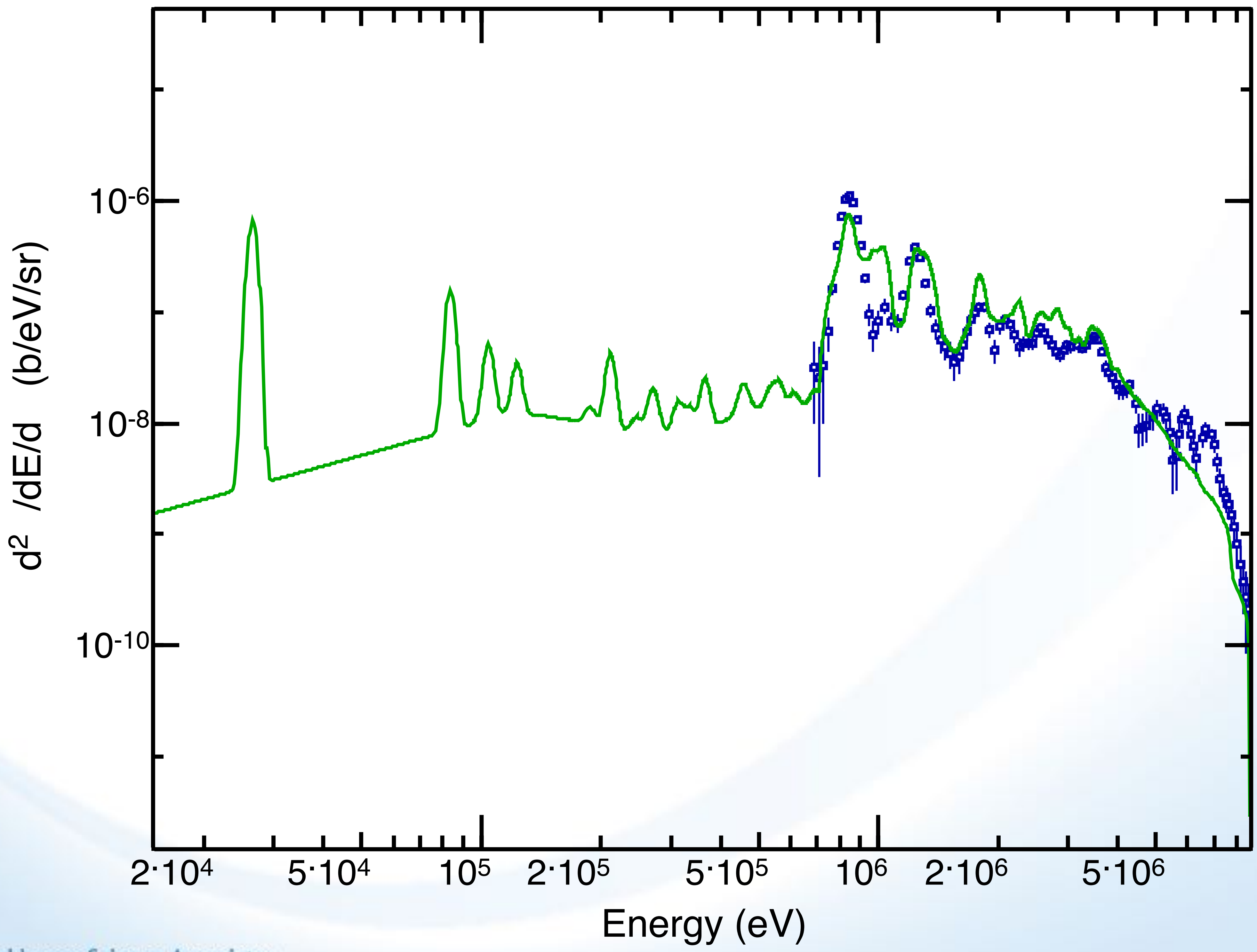
Complete discrete level decay schemes



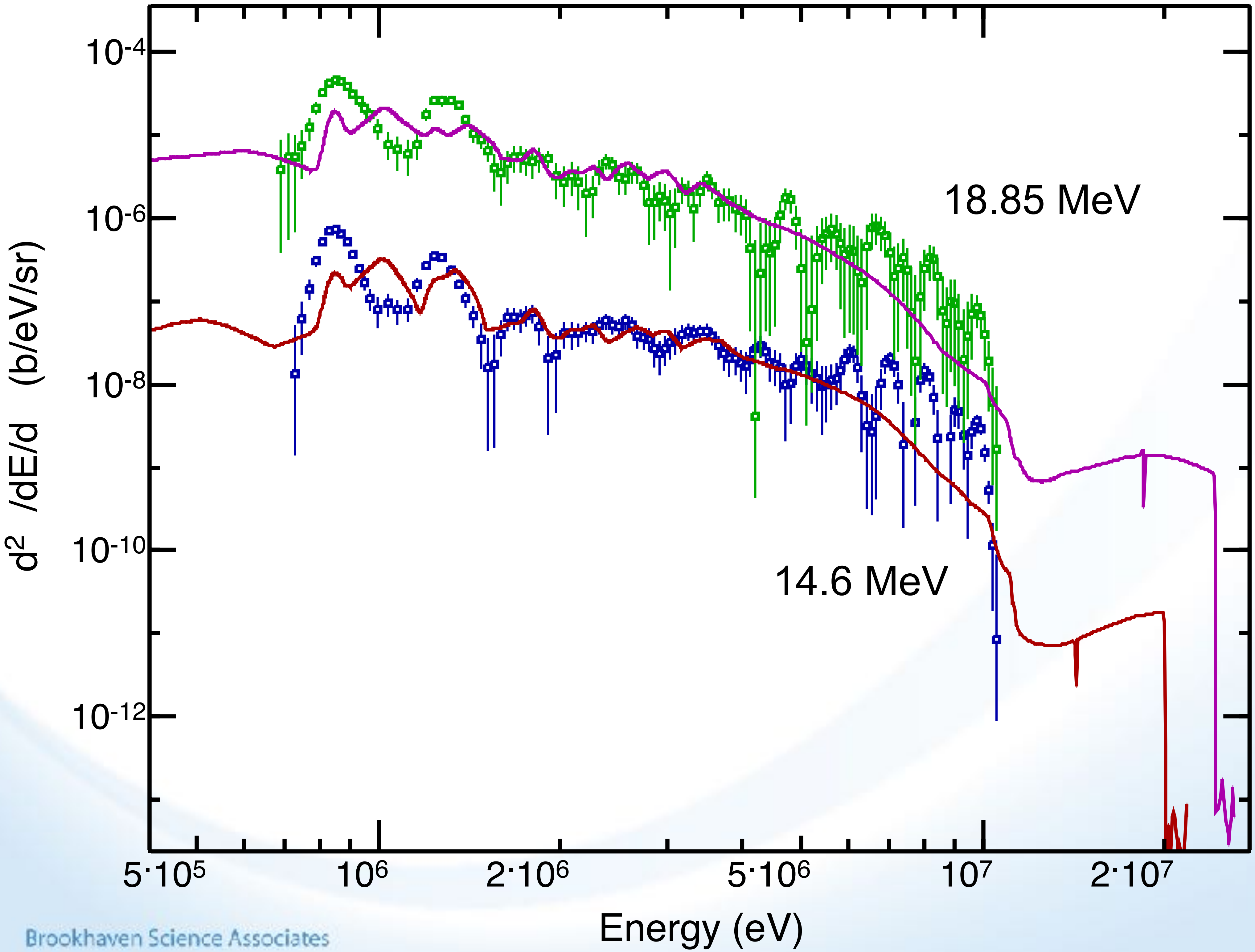
Still to be introduced in beta5



Gamma spectrum 56Fe(n,xγ) & 8.765 MeV, 125 deg



Gamma spectra 56Fe(n,xγ) at 14.6 & 18.85 MeV (125 deg)



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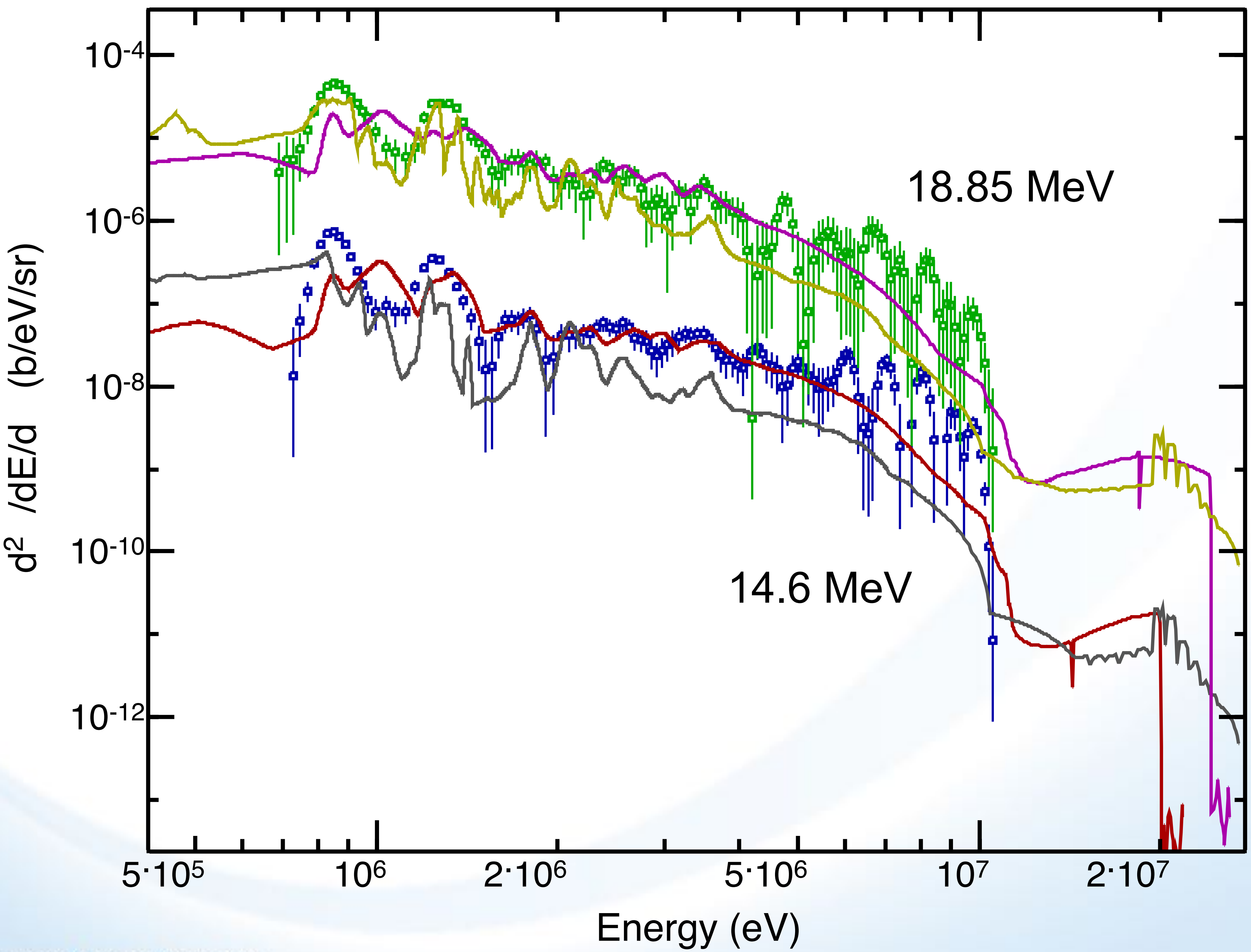
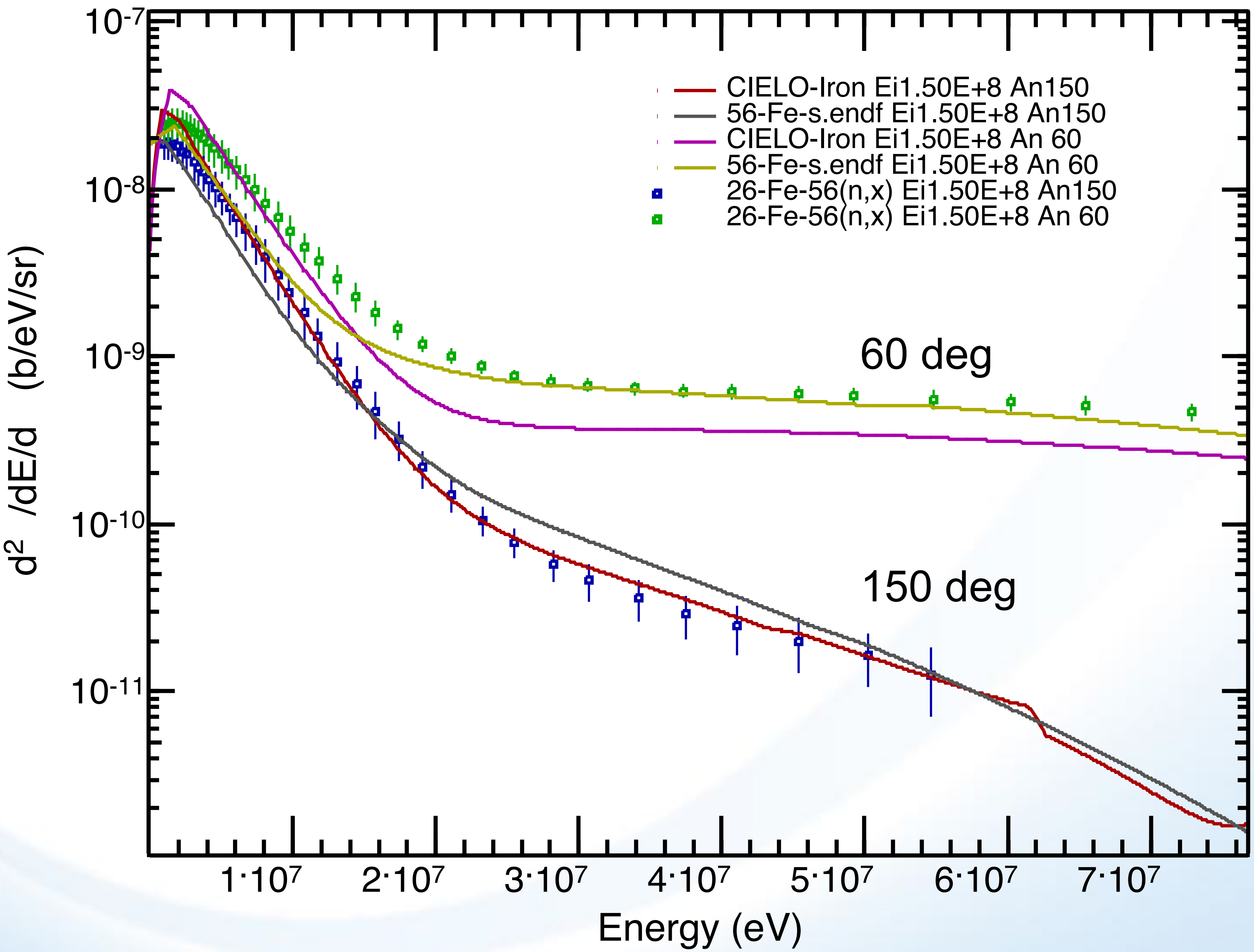
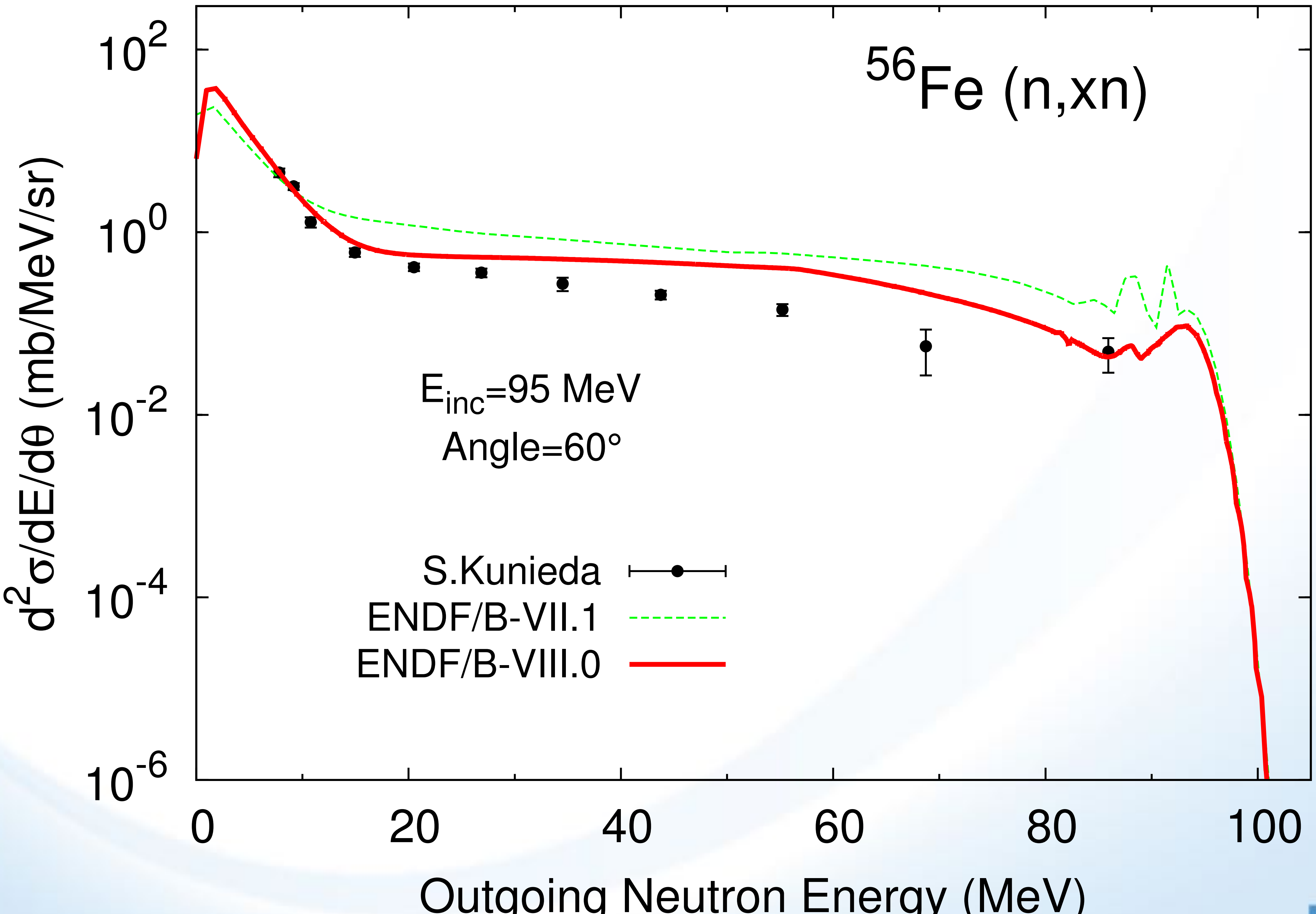


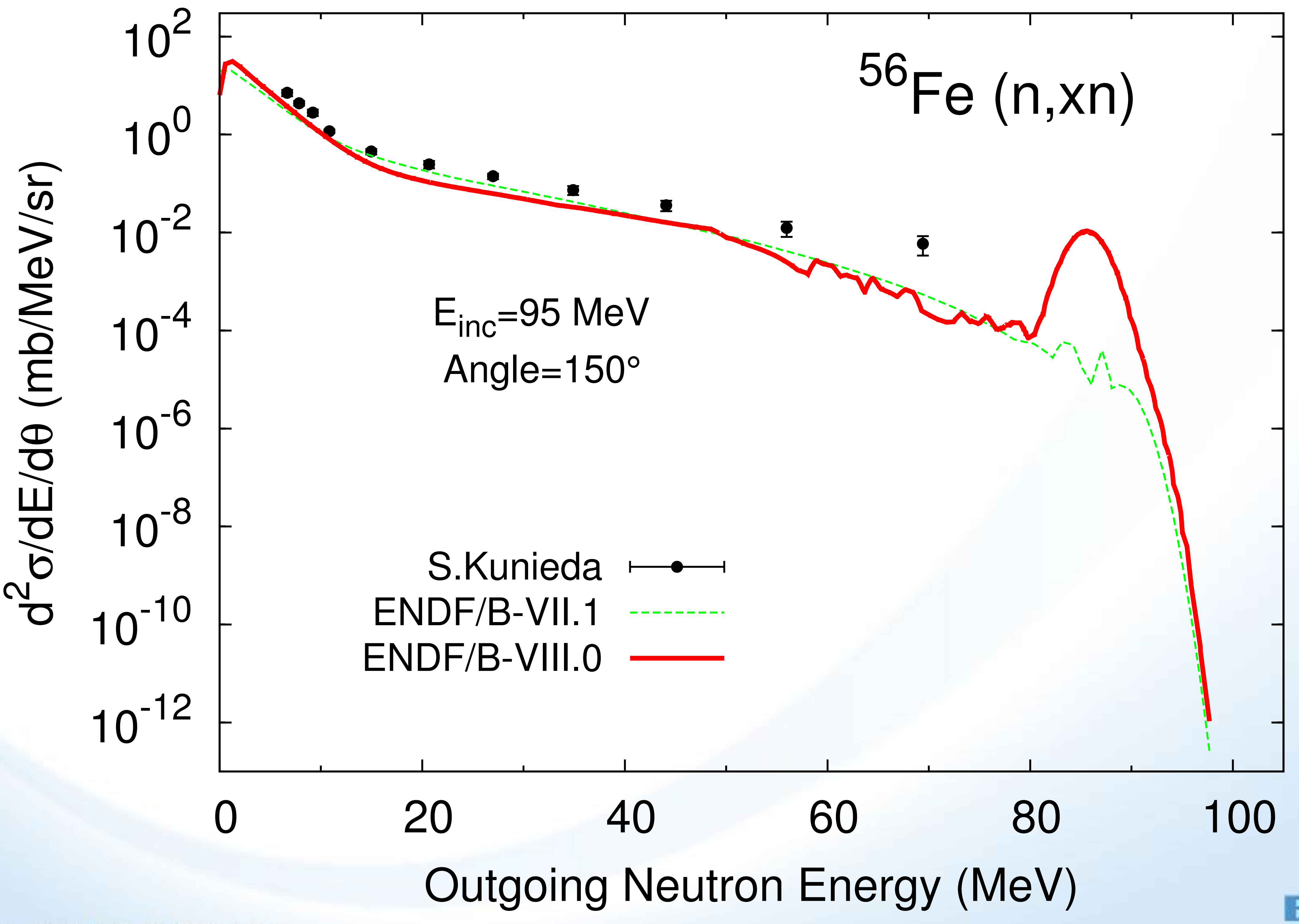
Neutron spectra from 56Fe at 150 MeV



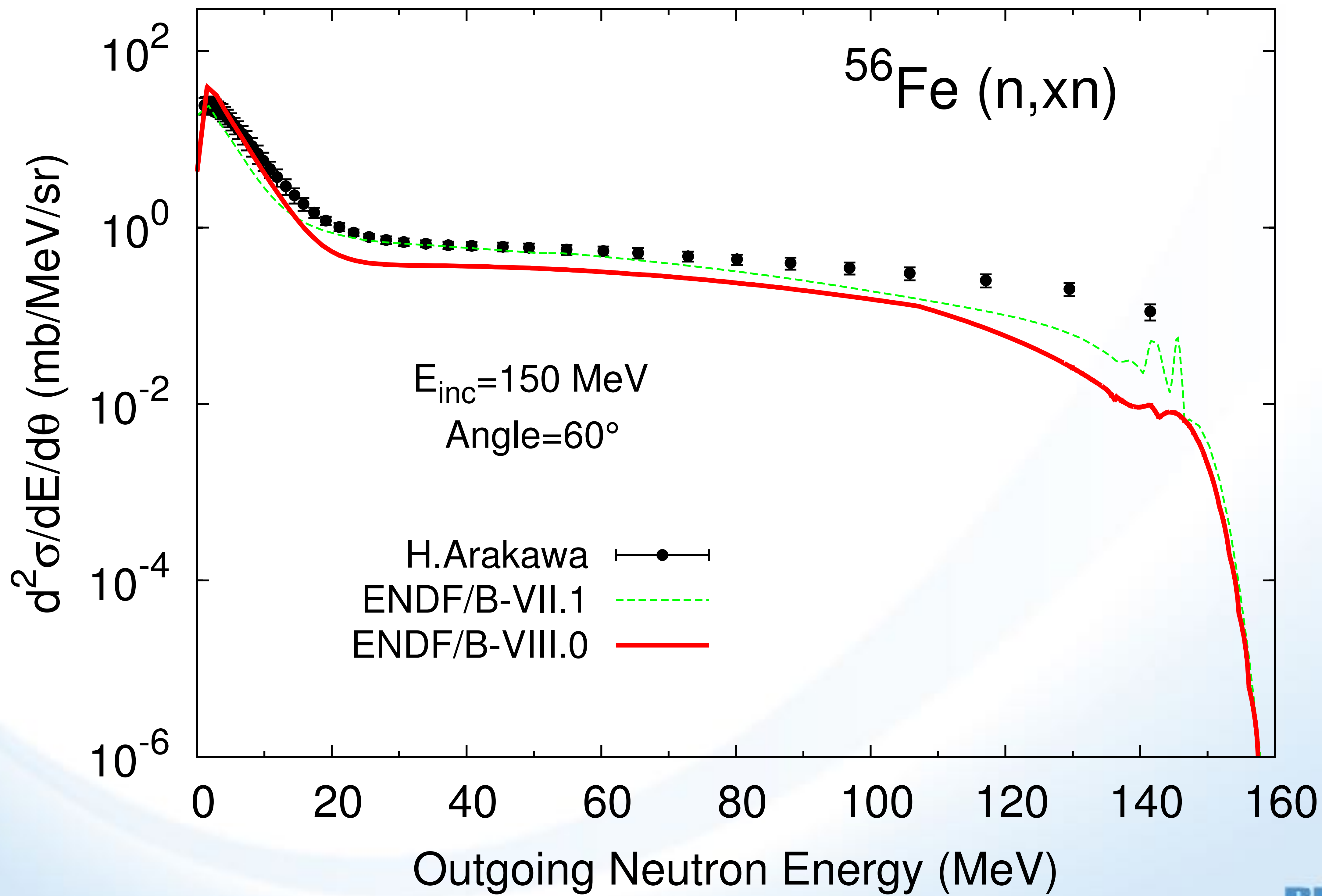
Neutron spectra from 56Fe at 95 MeV



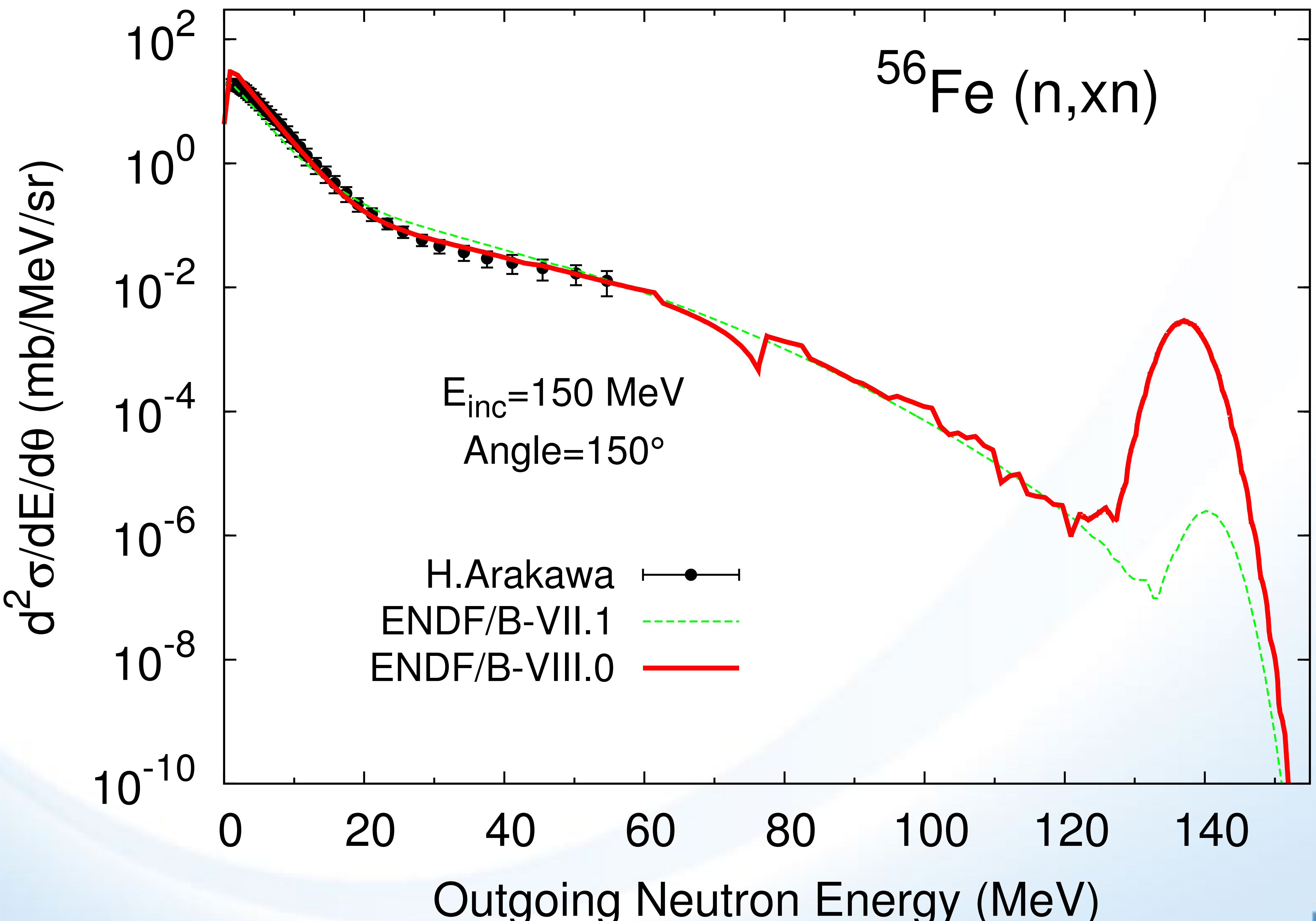
Neutron spectra from 56Fe at 150 MeV



Neutron spectra from 56Fe at 150 MeV



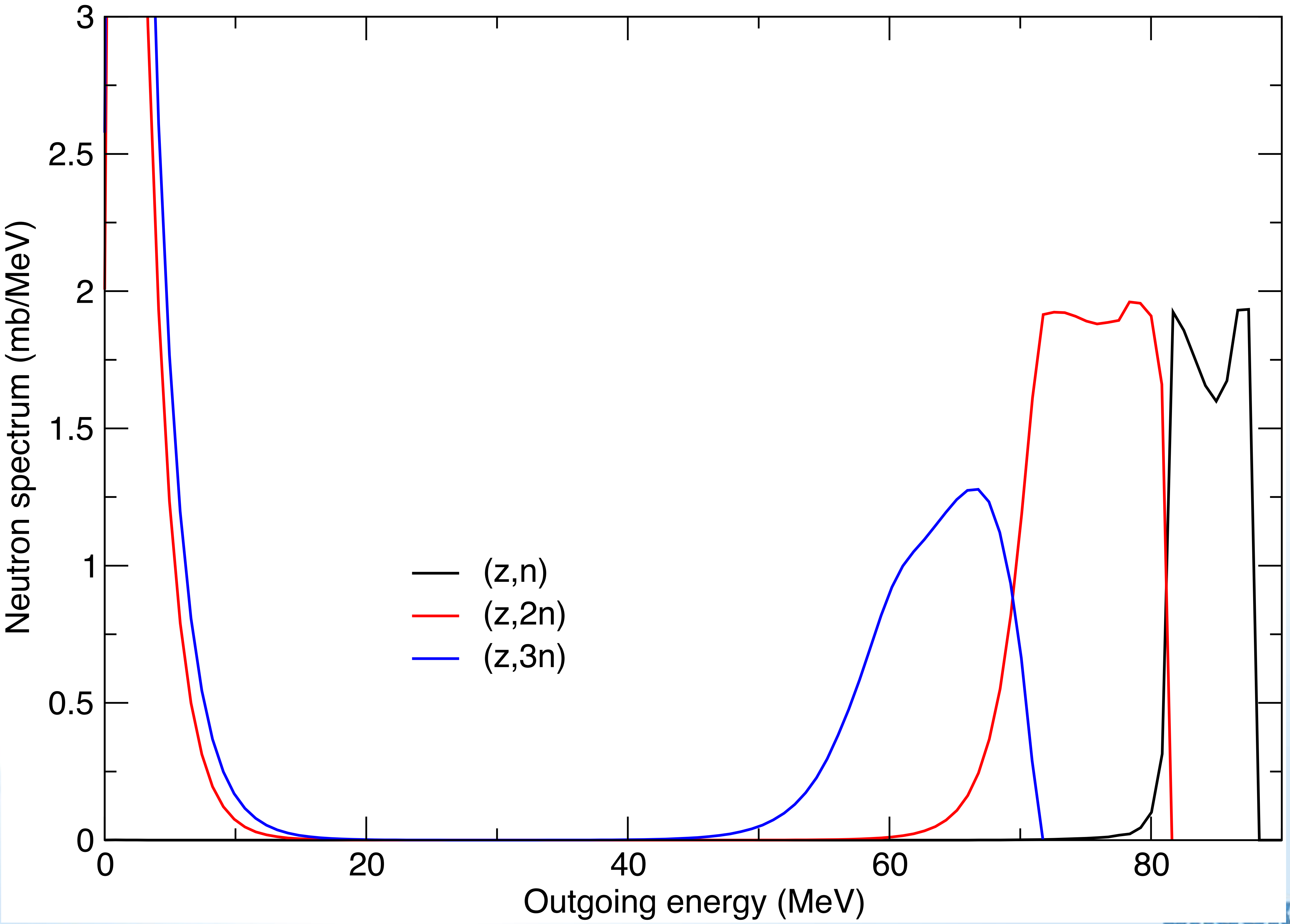
Neutron spectra from 56Fe at 150 MeV



Exclusive spectra

- ENDF-6 format requires that each reaction in MF=3 is accompanied by exclusive spectra (i.e., spectra being in coincidence with the production of the residue through the specific reaction)
- It is a tremendous challenge for the reaction model (unless it is Monte Carlo)
- EMPIRE includes algorithm to split usual emission spectra into exclusive spectra, with certain limitations:
  - splitting is done within Weisskopf-Ewing approximation
  - exclusive spectra are assigned to residues rather than reactions (not a problem for (n,xn) and (n,xp))
- They look… sort of odd and are a challenge for transport calculations

Exclusive spectra for $^{56}Fe(n,xn)$ at 96 MeV



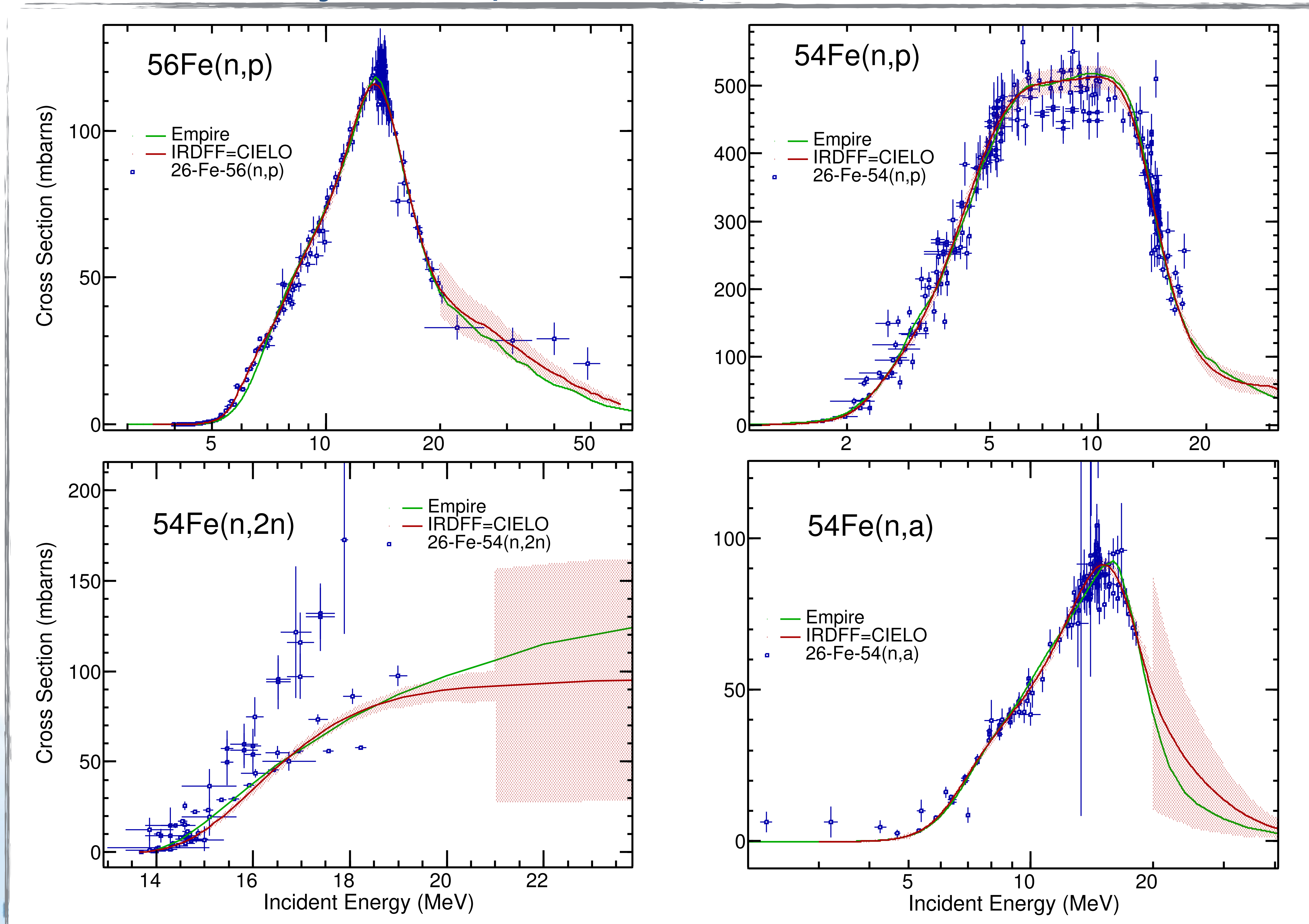
Minor Isotopes

^{54}Fe	RRR	Fast
β-2	• Evaluation based on Atlas up to 1.2 MeV • Improved several resonances	• Capture artificially scaled down across the board in an attempt to improve matching with resonance region
β-3	• IRSN resonances up to 1.036 MeV	• Better fit of (n,p), (n,a), (n,2n) to IRDFF evaluation • Energy-dependent scaling of total in order to reproduce Guenther elastic data below 2 MeV and improve agreement with ave. VII.1 between 700 keV and 1.2 MeV • Restored capture from Beta 1 and then lowered it to agree with low-lying Allen data

^{57}Fe	RRR	Fast
β-2	• New LRF=7 evaluation from Atlas • Converted from MLBW to Reich-Moore LRF=7 to include first inelastic	• Gilbert-Cameron level densities
β-3	• Same as β-2	• Corrected coupled and DWBA levels • HMS

^{58}Fe	RRR	Fast
β-3=β-2	• Moxon evaluation	• EMPIRE

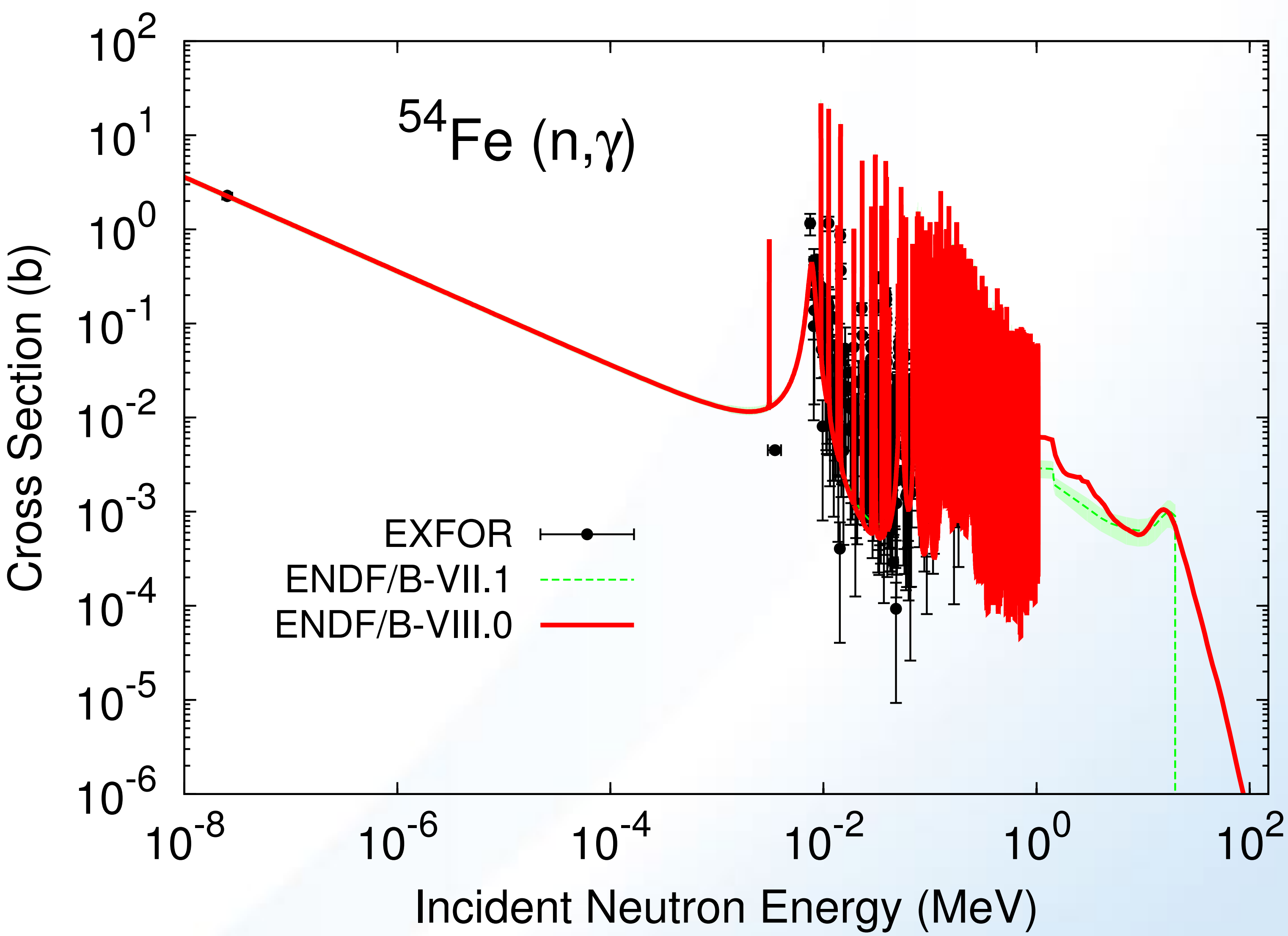
Dosimetry file (IRDFF)



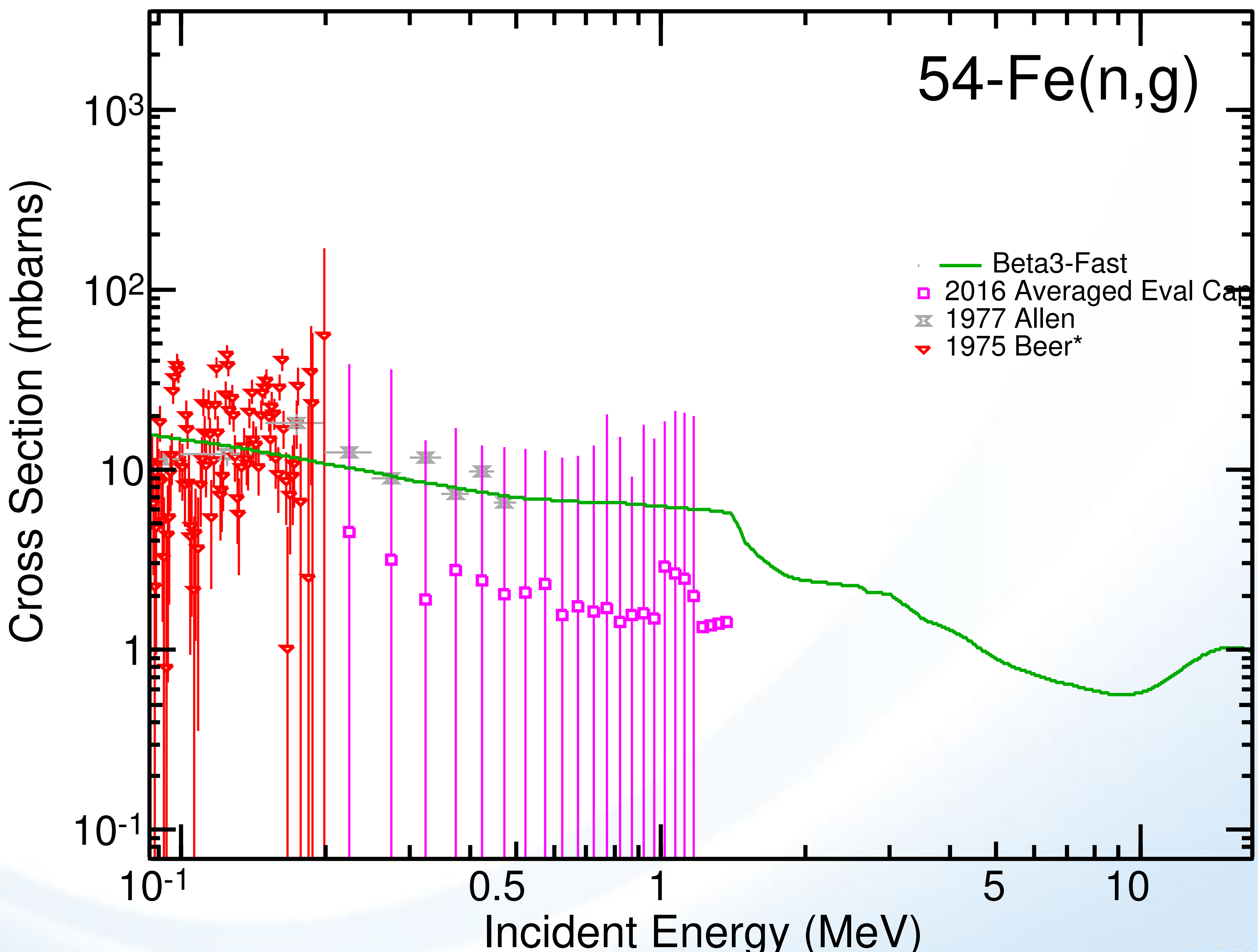
Changes in ^{54}Fe evaluation (β3 => β4)

Adding 64 resonances

- G. Giubrone's thesis "Neutron capture measurement of 54Fe and 57Fe at CERN n_TOF", University of Valencia (2014), noted in Atlas evaluation but missing from IRSN evaluation



^{54}Fe capture issue



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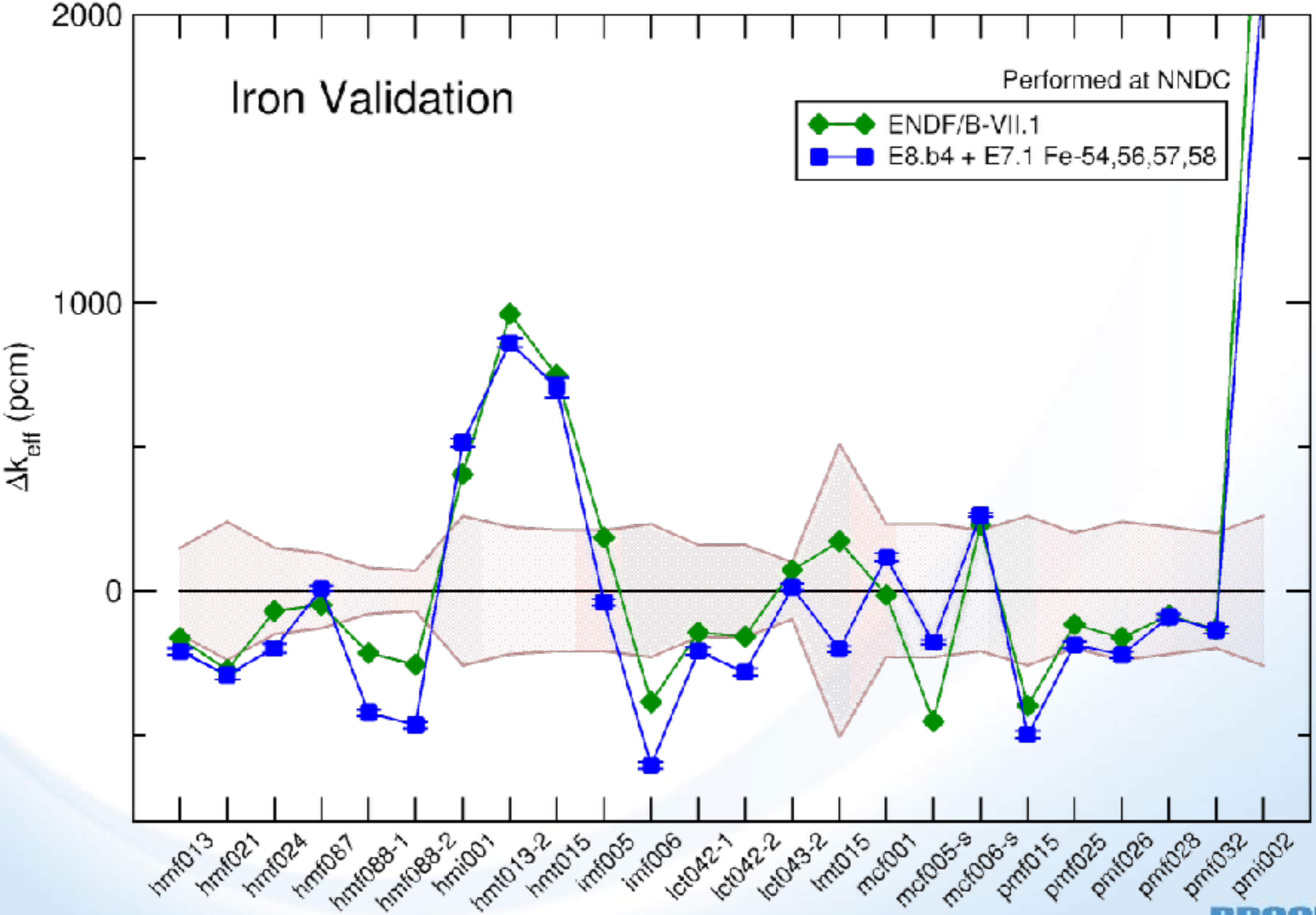
Validation: the effect of β4 (keeping VII.1 Fe)



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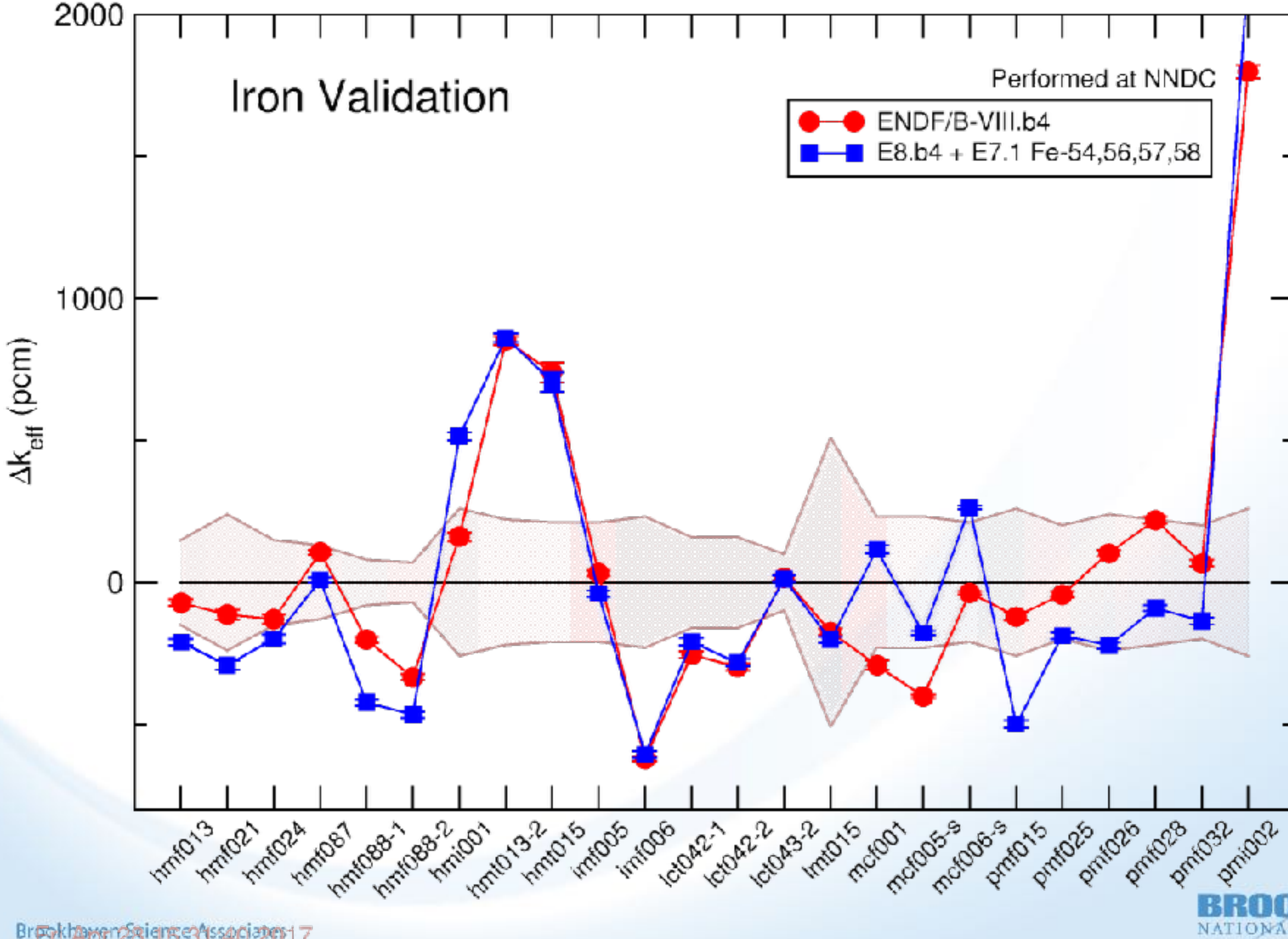
Validation: the effect of β4 Fe



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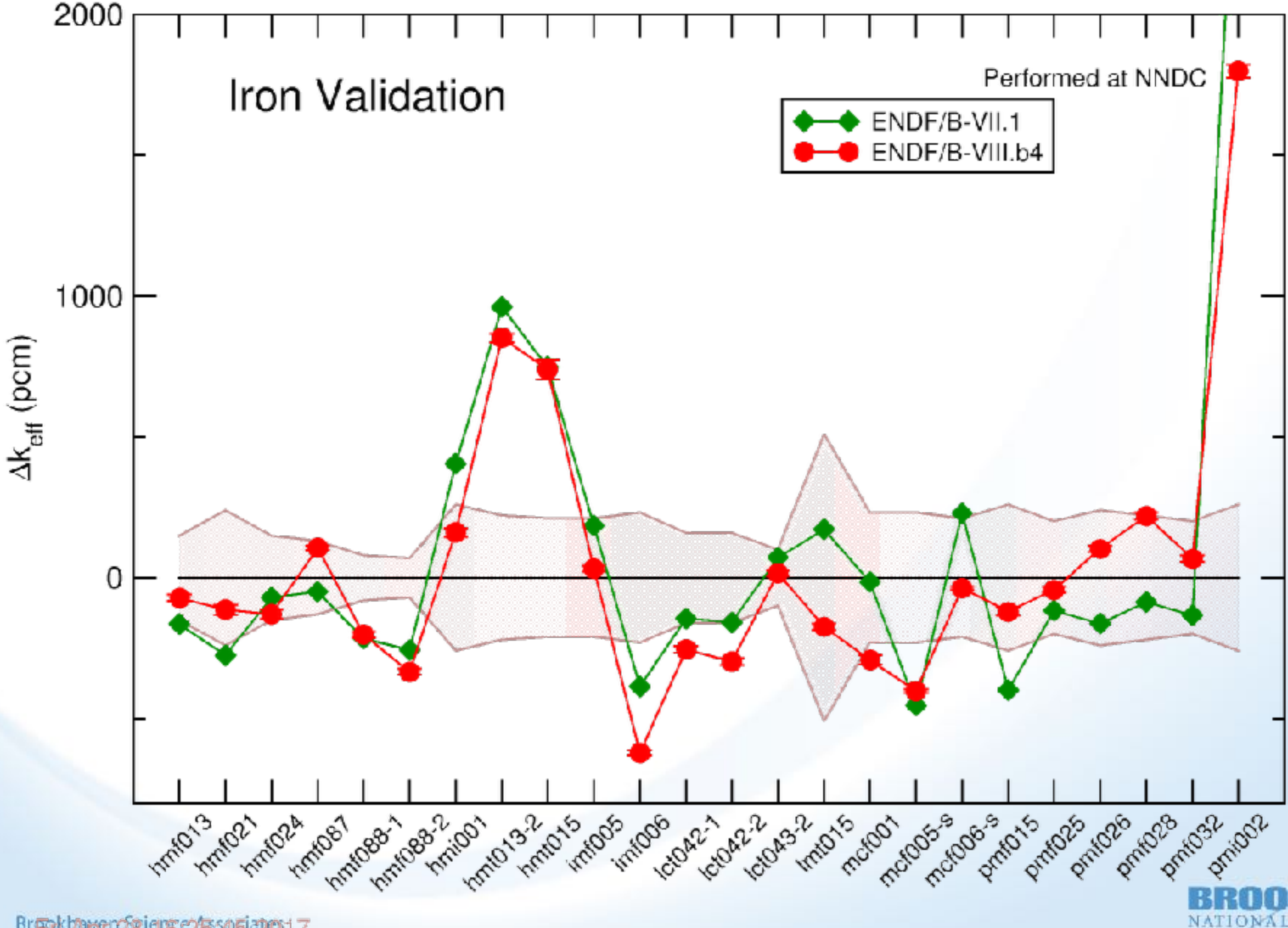
Validation: VII.1 versus β4



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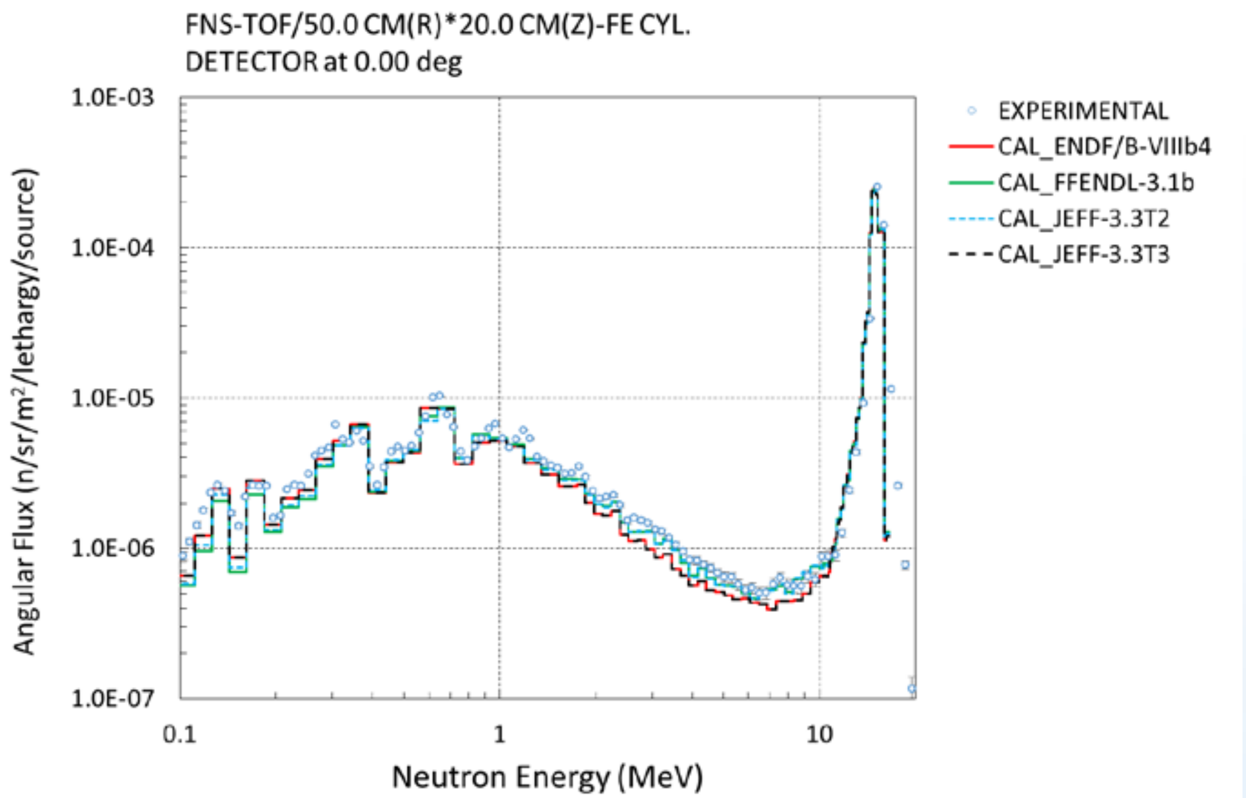
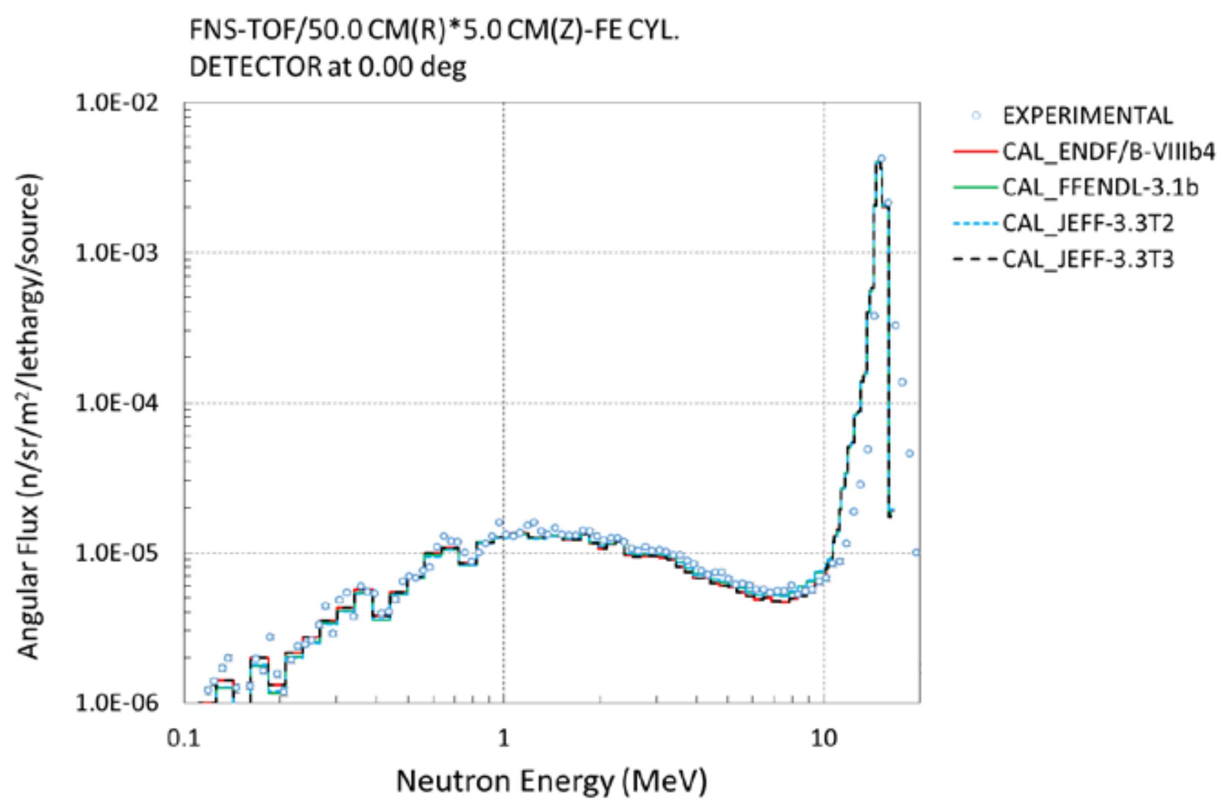
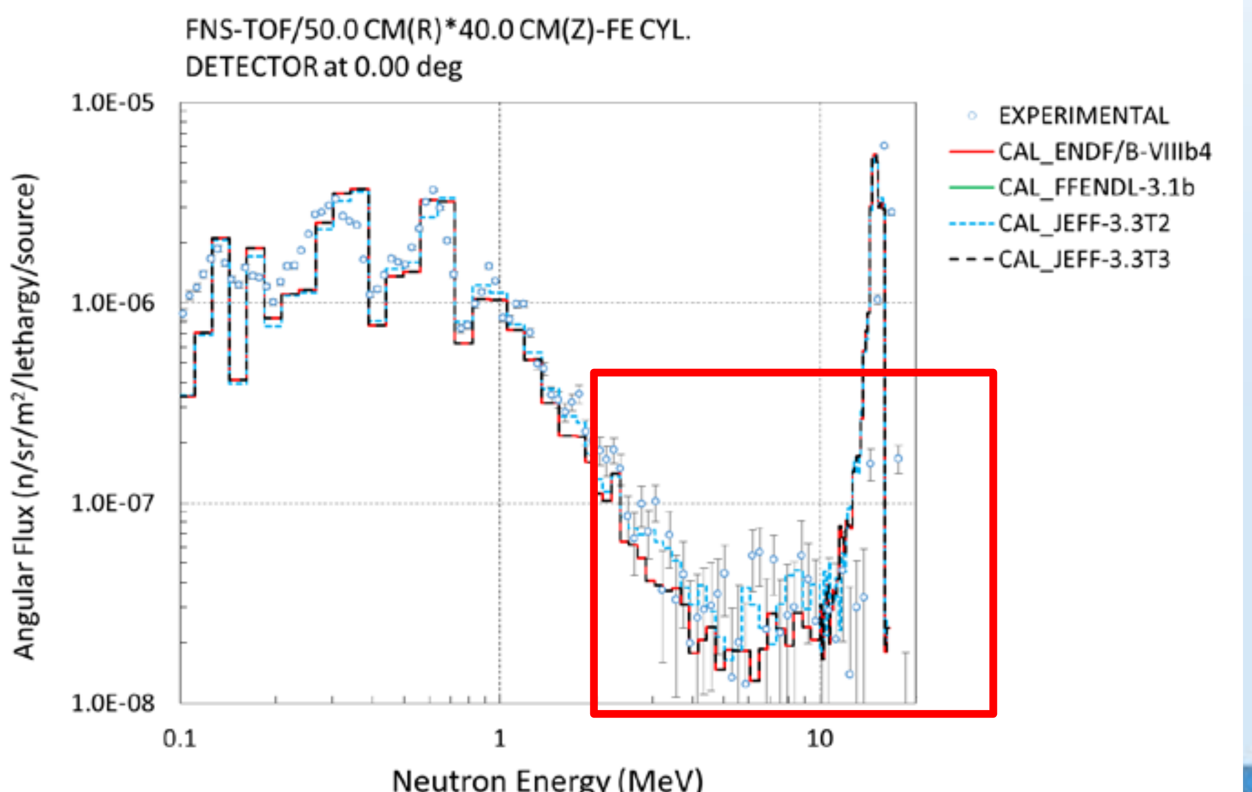
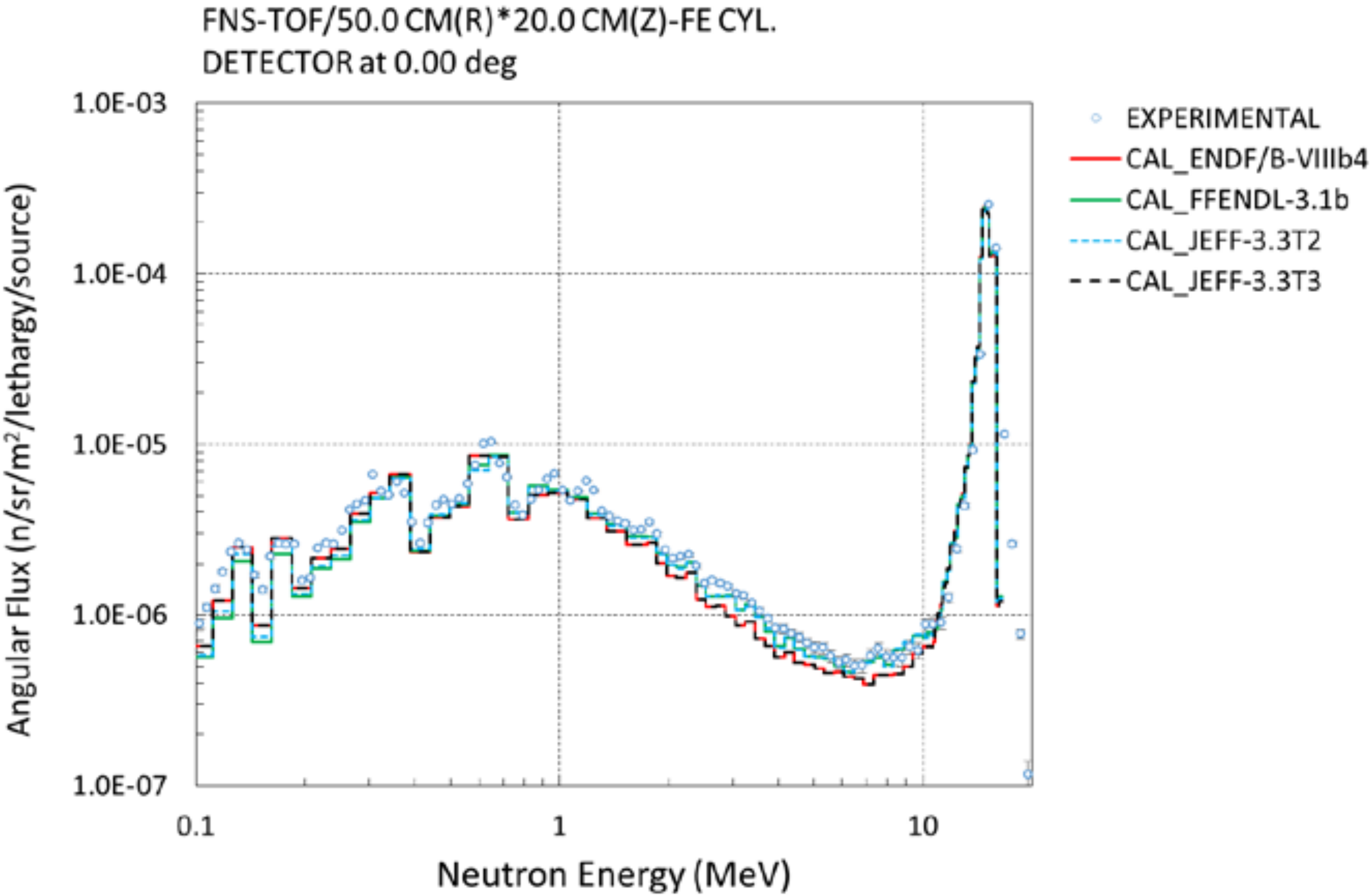
Figures. Results obtained for the **<u>Fe (iron)</u>** ToF-experiment at FNS showing angular neutron leakage spectra for thick slabs <u>at 0 degrees</u>

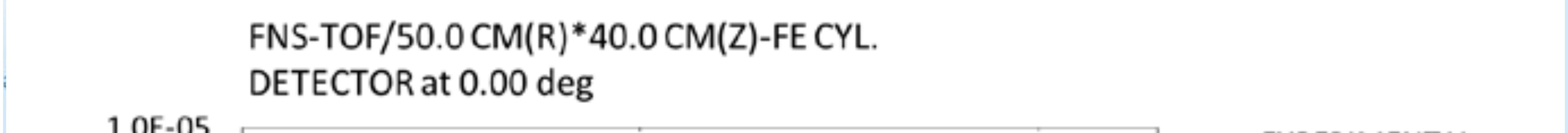
- Fe, slightly better agreement in JEFF-3.3T2

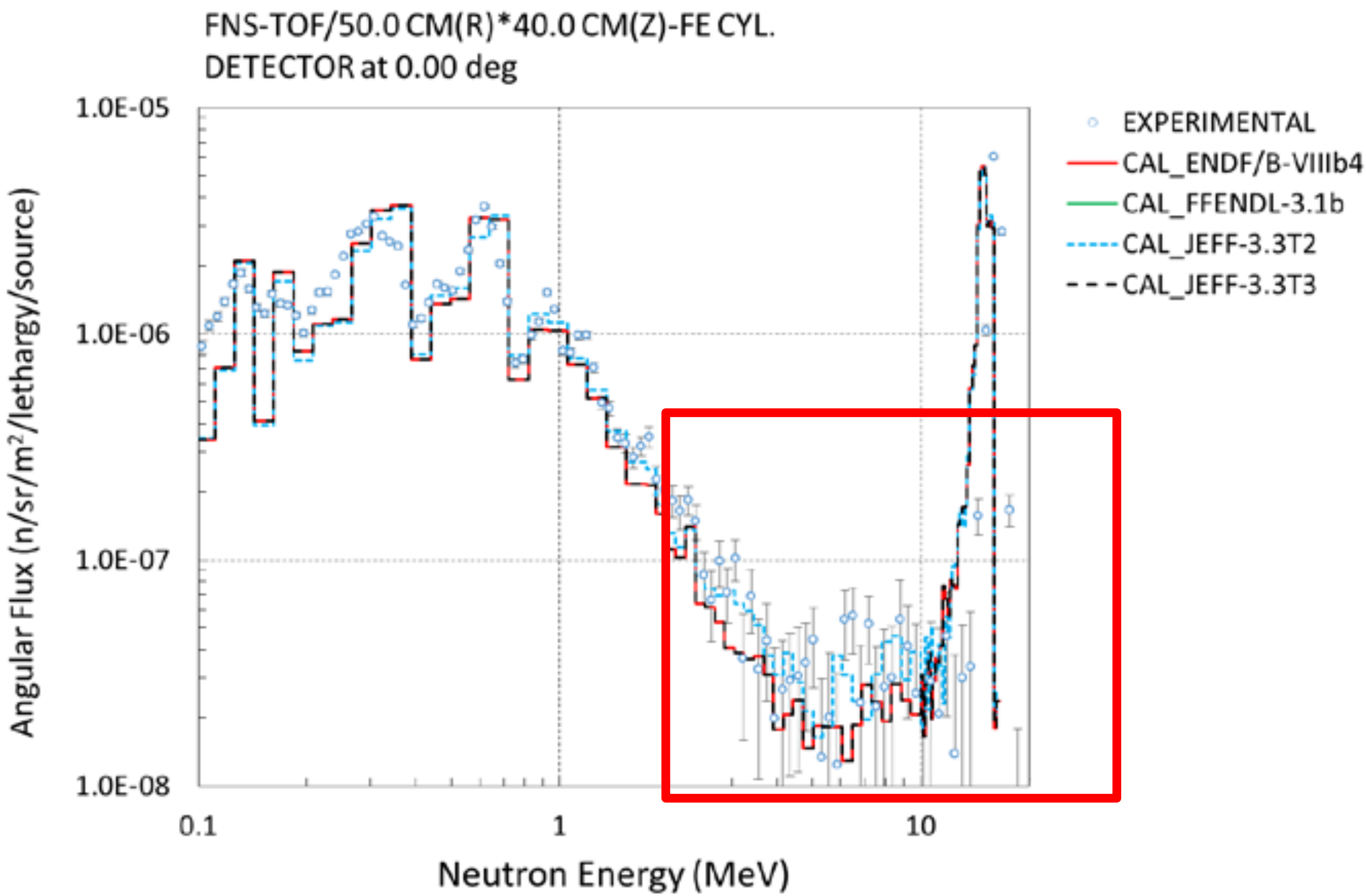




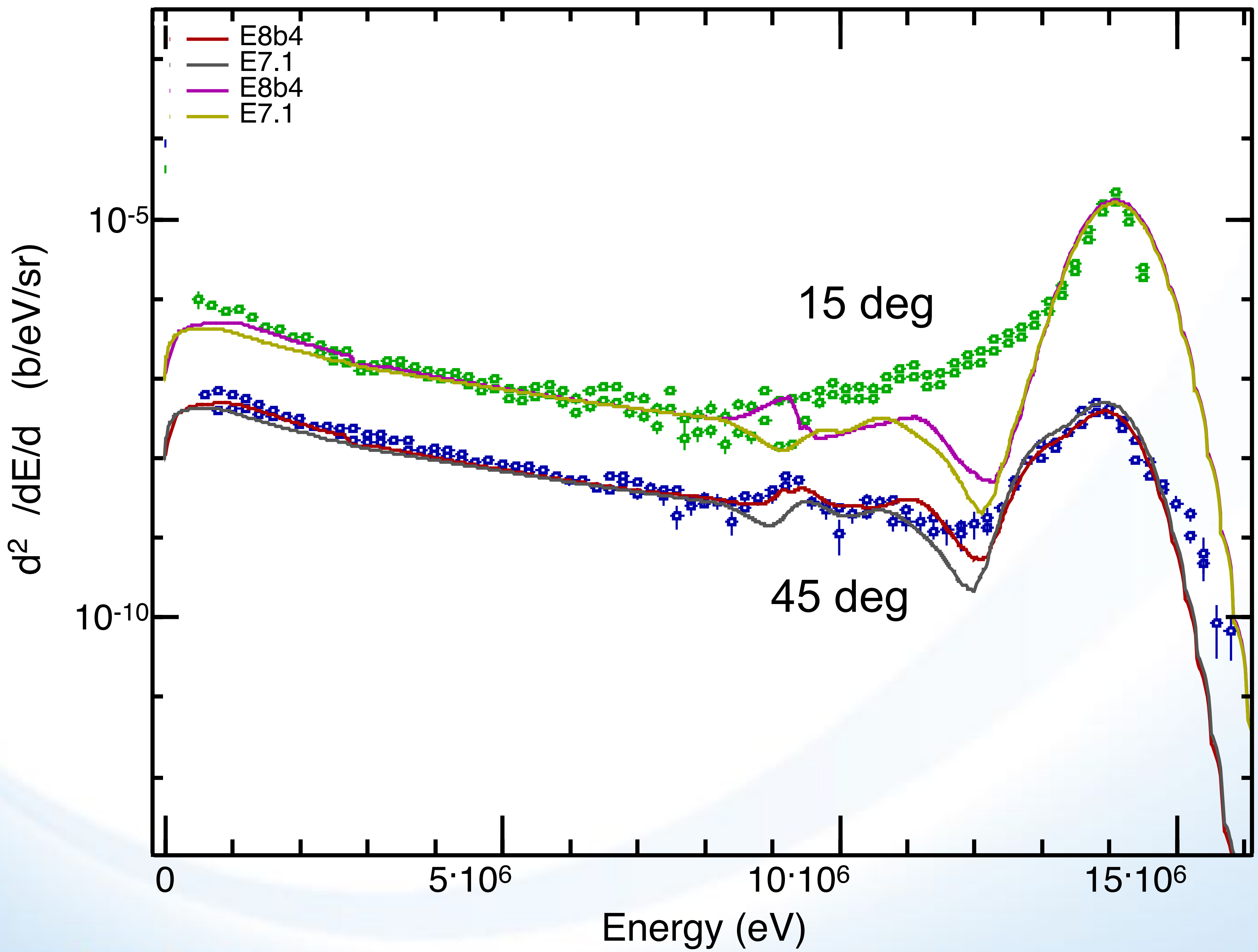



FNS-TOF/50.0 CM(R)*20.0 CM(Z)-FE CYL.
DETECTOR at 0.00 deg
Angular Flux (n/sr/m²/lethargy/source)
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
0.1
1
10
Neutron Energy (MeV)
EXPERIMENTAL
CAL_ENDF/B-VIIIb4
CAL_FFENDL-3.1b
CAL_JEFF-3.3T2
CAL_JEFF-3.3T3

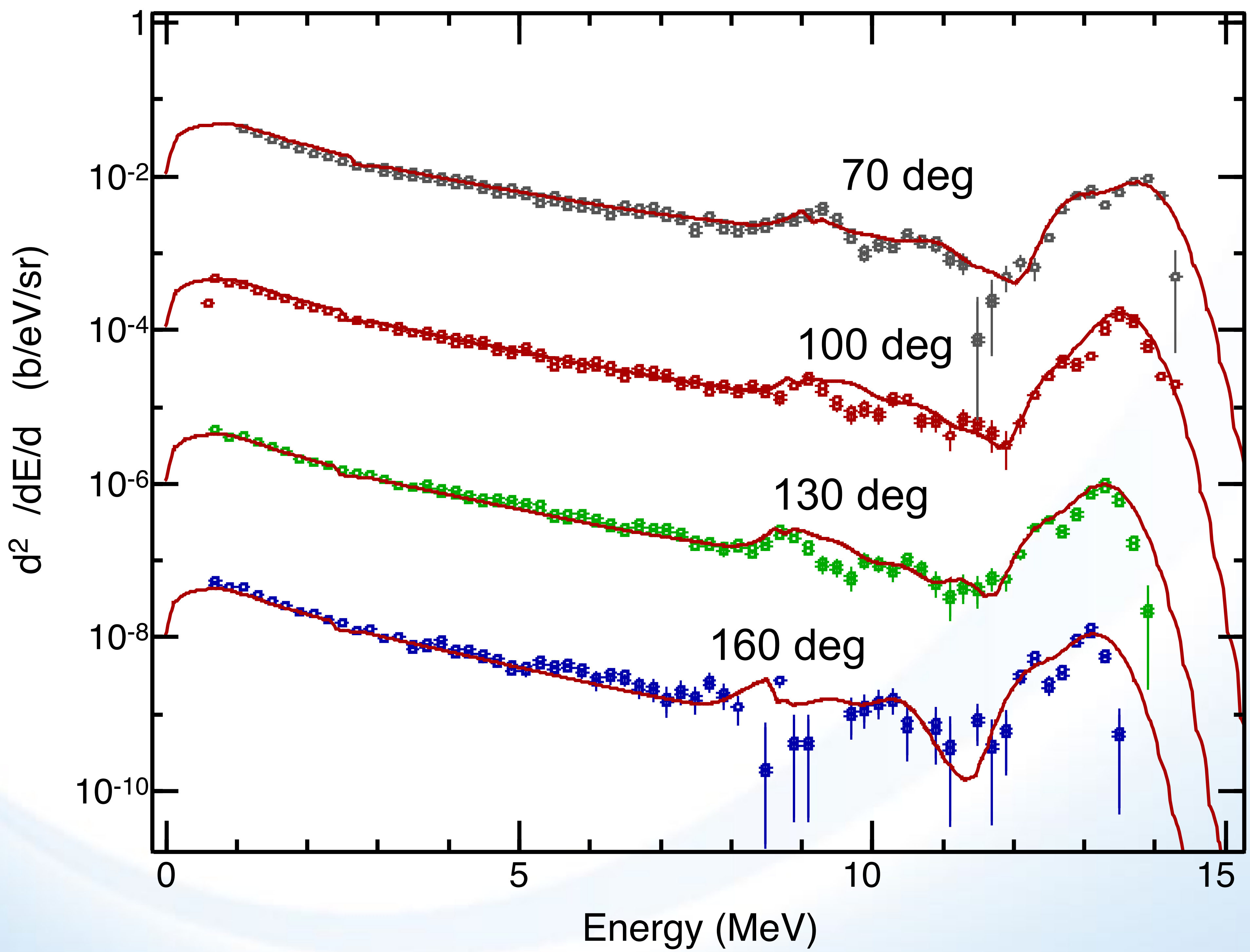

FNS-TOF/50.0 CM(R)*40.0 CM(Z)-FE CYL.
DETECTOR at 0.00 deg


FNS-TOF/50.0 CM(R)*40.0 CM(Z)-FE CYL.
DETECTOR at 0.00 deg
1.0E-05
1.0E-06
1.0E-07
1.0E-08
0.1
1
10
Angular Flux (n/sr/m²/lethargy/source)
Neutron Energy (MeV)
EXPERIMENTAL
CAL_ENDF/B-VIIIb4
CAL_FFENDL-3.1b
CAL_JEFF-3.3T2
CAL_JEFF-3.3T3

$^{56}Fe(n,xn)$ ddx spectra at E_{inc}=14.1



$^{56}Fe(n,xn)$ ddx spectra at $E_{inc}=14.1$



Still to do…

- Try to improve DWBA calculations
  - improve performance in shielding experiments
  - improve inelastic gammas
  - improve gamma spectra
  - maintain neutron ddx above 30 deg
- COVARIANCES