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International Atomic Energy Agency
Atoms for Peace and Development

IAEA-INDEN (Post-CIELO) ^{56}Fe Evaluation and Benchmarking

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CIELO ^{56}Fe evaluation adopted for ENDF-/B-VIII.0 (+ $^{54,57,58}\text{Fe}$)



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Evaluation of Neutron Reactions on Iron Isotopes for CIELO and ENDF/B-VIII.0

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Background

- The ENDF/B-VIII.0 adopted the CIELO evaluation for ^{56}Fe .
- Deficiencies were revealed in the ^{56}Fe CIELO evaluation just before the release of the ENDF/B-VIII.0 library
- Work is in progress to remove the deficiencies.

Problems with CIELO ^{56}Fe

- It was noted during benchmarking of the ENDF/B-VIII.0 library that leakage spectra from thick iron shells with ^{252}Cf source and with D-T source were poorly reproduced (reported by S. Simakov).
- The problem was traced to the non-elastic cross section that could be too high in some energy regions (some impact of ang. distr.).
- There were also minor fixes to the elastic cross sections in the resonance region

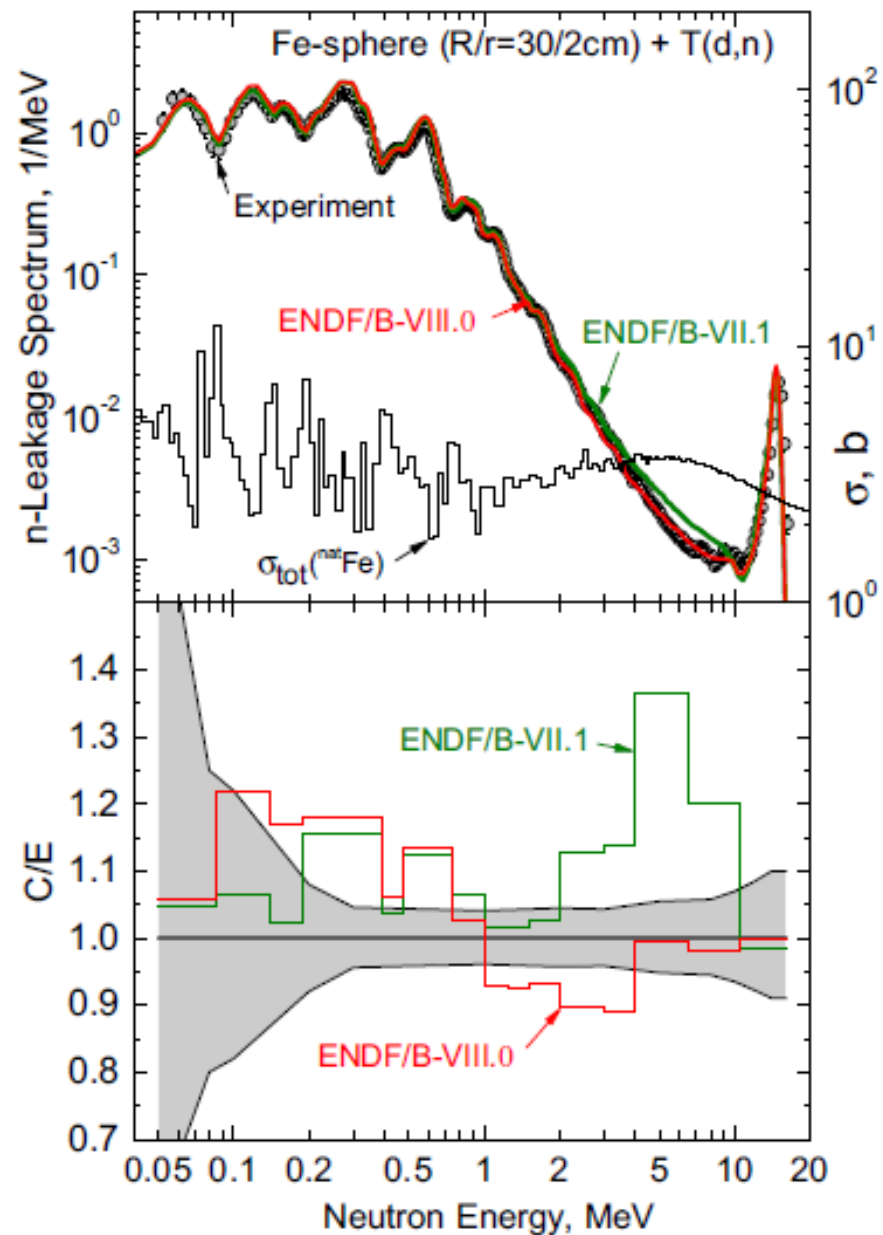
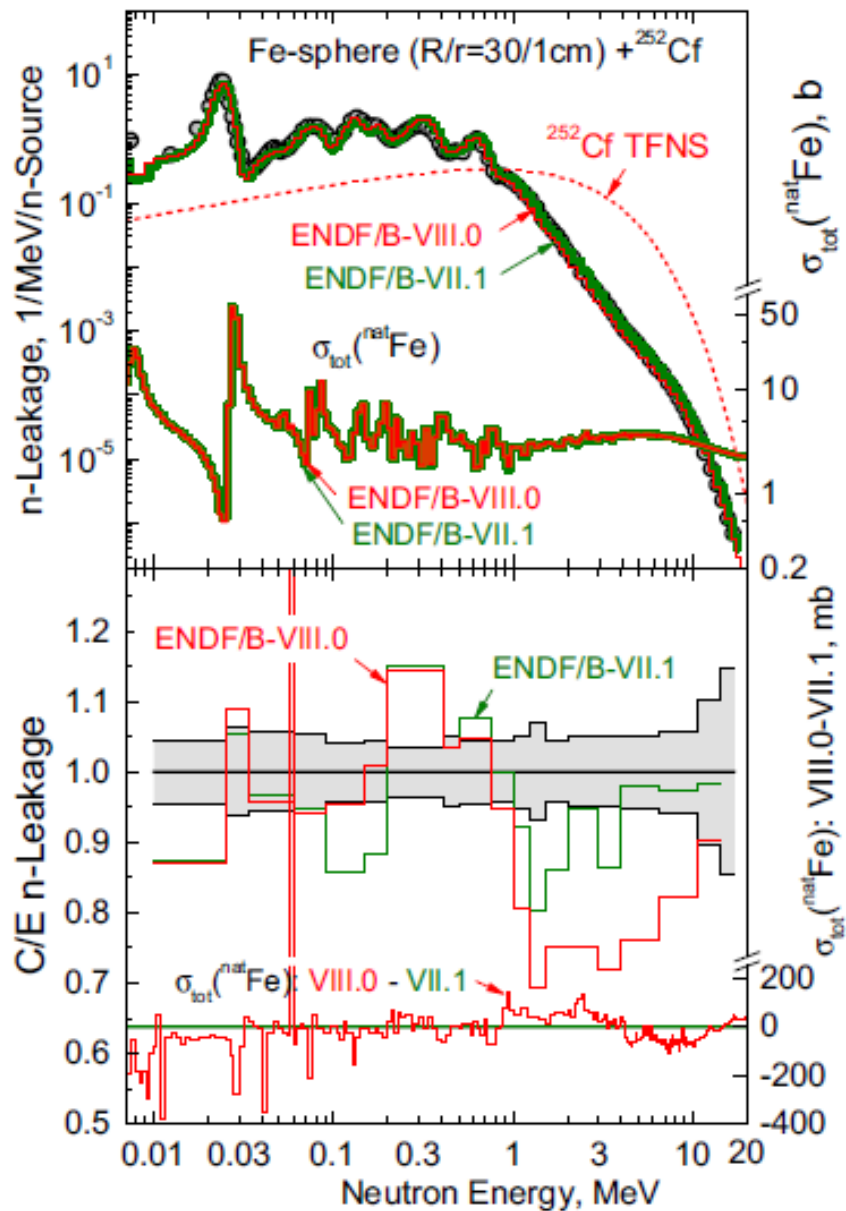


Fig. 32, 35, Nuclear Data Sheets, 148 (2018) 214-253

Improvements to ^{56}Fe evaluation

- Total cross sections above 2 MeV are trusted.
- New measurements by E. Pirovano at JRC Geel support a higher elastic cross section.
- Capture is too small to play a role.
→ **Hypothesis: inelastic is too high at least above 2 MeV where measurements of the elastic x.s. are available.**
- Inelastic cross section was scaled down to the lowest bound of uncertainty, assigning the difference to elastic (exact comparison of cross sections is difficult due to strong fluctuations).
- Small changes to the total cross section below 2 MeV.
- Small corrections to the elastic cross section in the resonance interference minima (e.g., near 300 keV)
- Thermal capture reduced by 10%
(Firestone et al, PRC **95**(2017) 014328)

Experimental data used below 4 MeV:



Differential experiments:

- ✓ High resolution σ_{tot} , σ_{inl}
- ✓ Lower resolution σ_{inl}
- ✓ Elastic cross sections (AD)
- ✓ High resolution AD (Kinney et al, Perey et al.)

Integral experiments:

- ✓ Criticality assemblies
- ✓ Cf-252(sf) shielding benchmarks
- ✓ DT shielding benchmarks
- ✓ SACS in well defined neutron spectra

Differential experiments: σ_{inl}

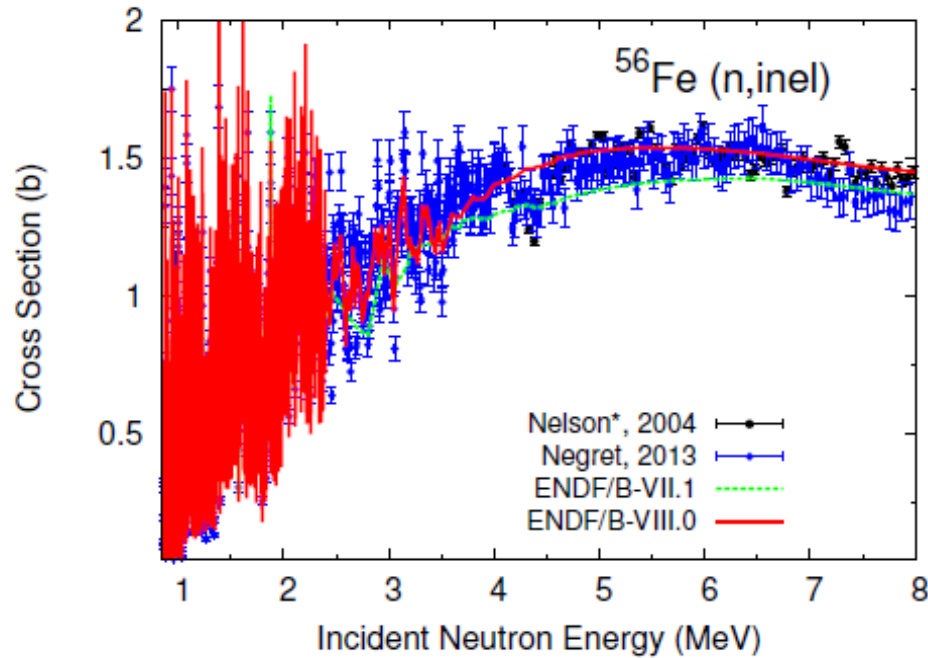


FIG. 34. (Color online) Evaluated $^{56}\text{Fe}(n, n')$ neutron inelastic cross section compared with data retrieved from EXFOR and with the previous evaluation. The asterisk on the Nelson data indicates that they are renormalized as described in Ref. [19].

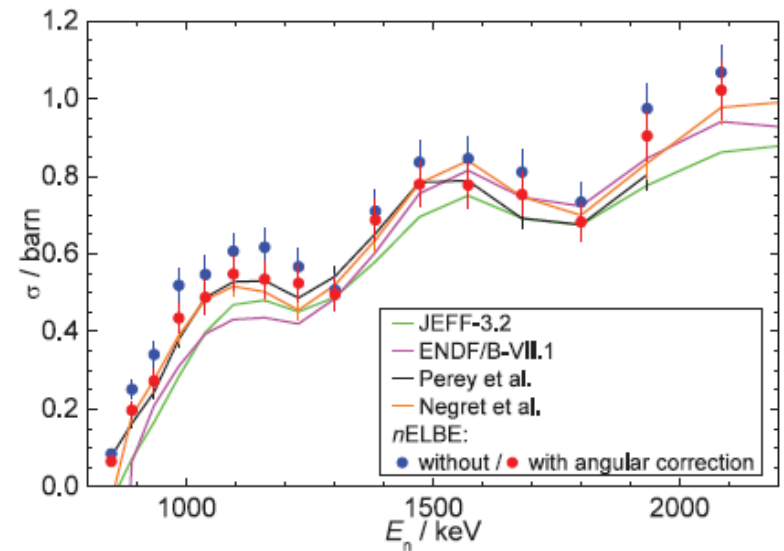
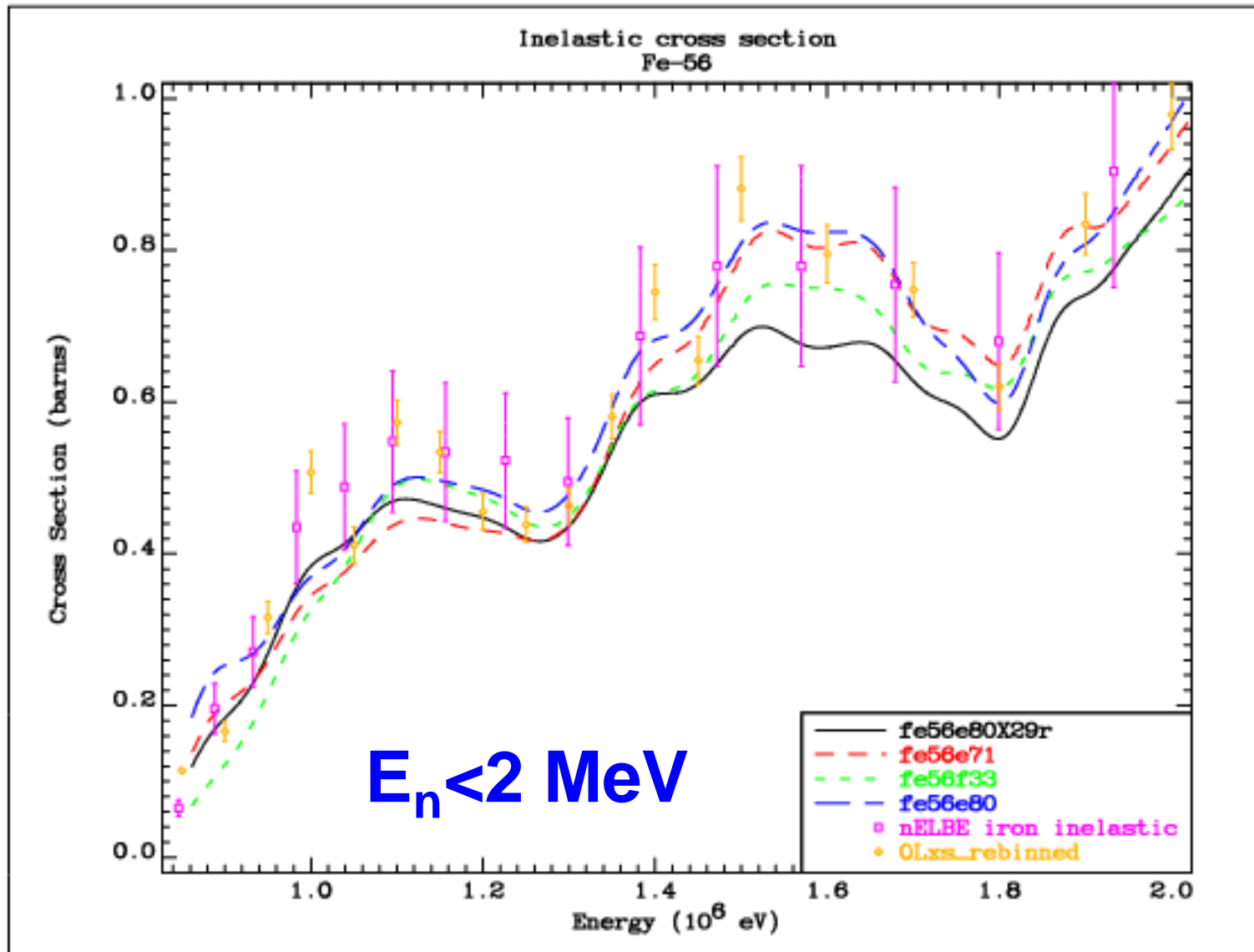


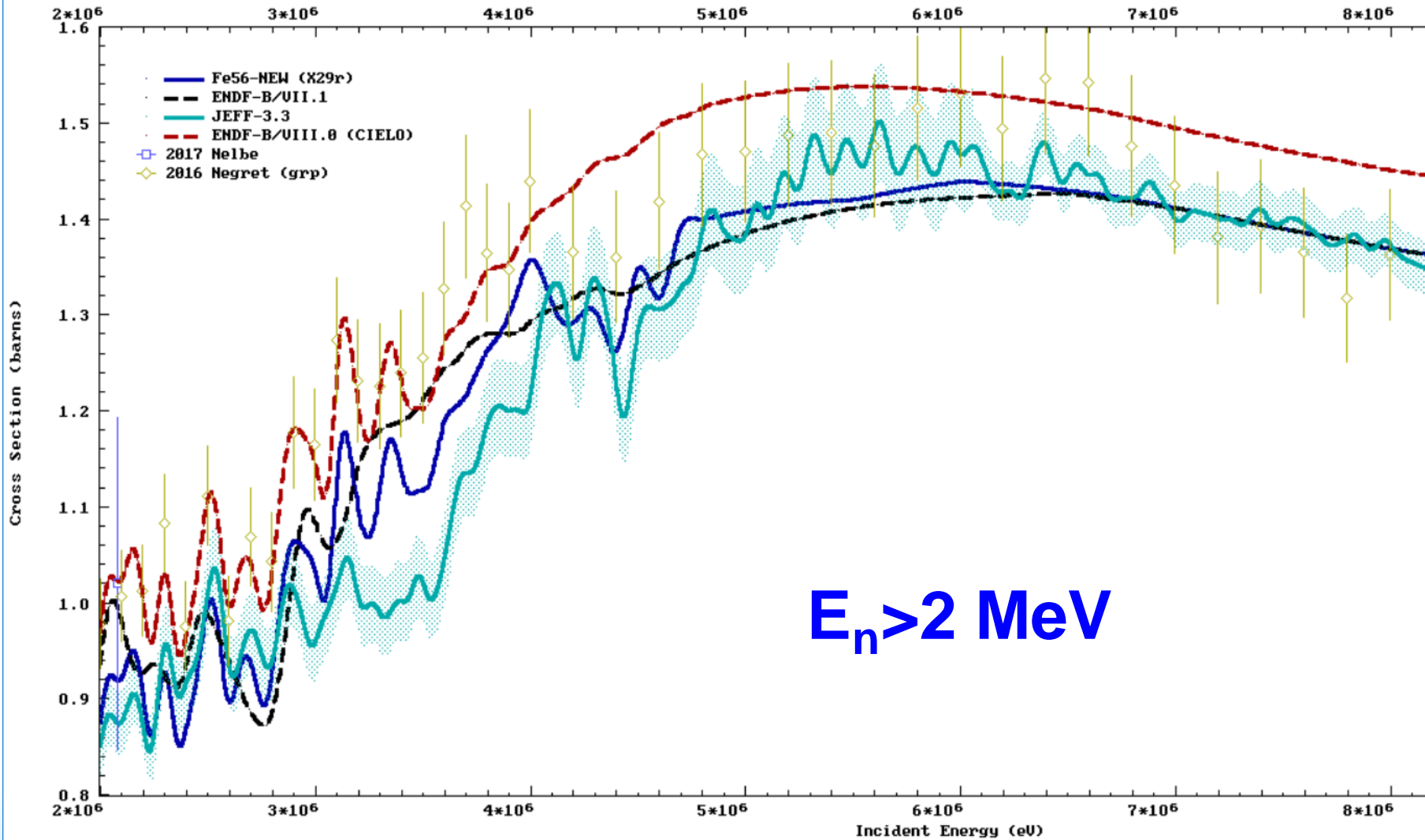
Figure 9. Inelastic neutron scattering cross section under excitation of the first excited state of ^{56}Fe determined in the γ -ray production measurement before and after correction for the γ -ray angular distribution. (Note: The reference data are averaged to the binsize of the n ELBE measurement.)

Beyer et al, EPJ WoC 146 (2017) 02017

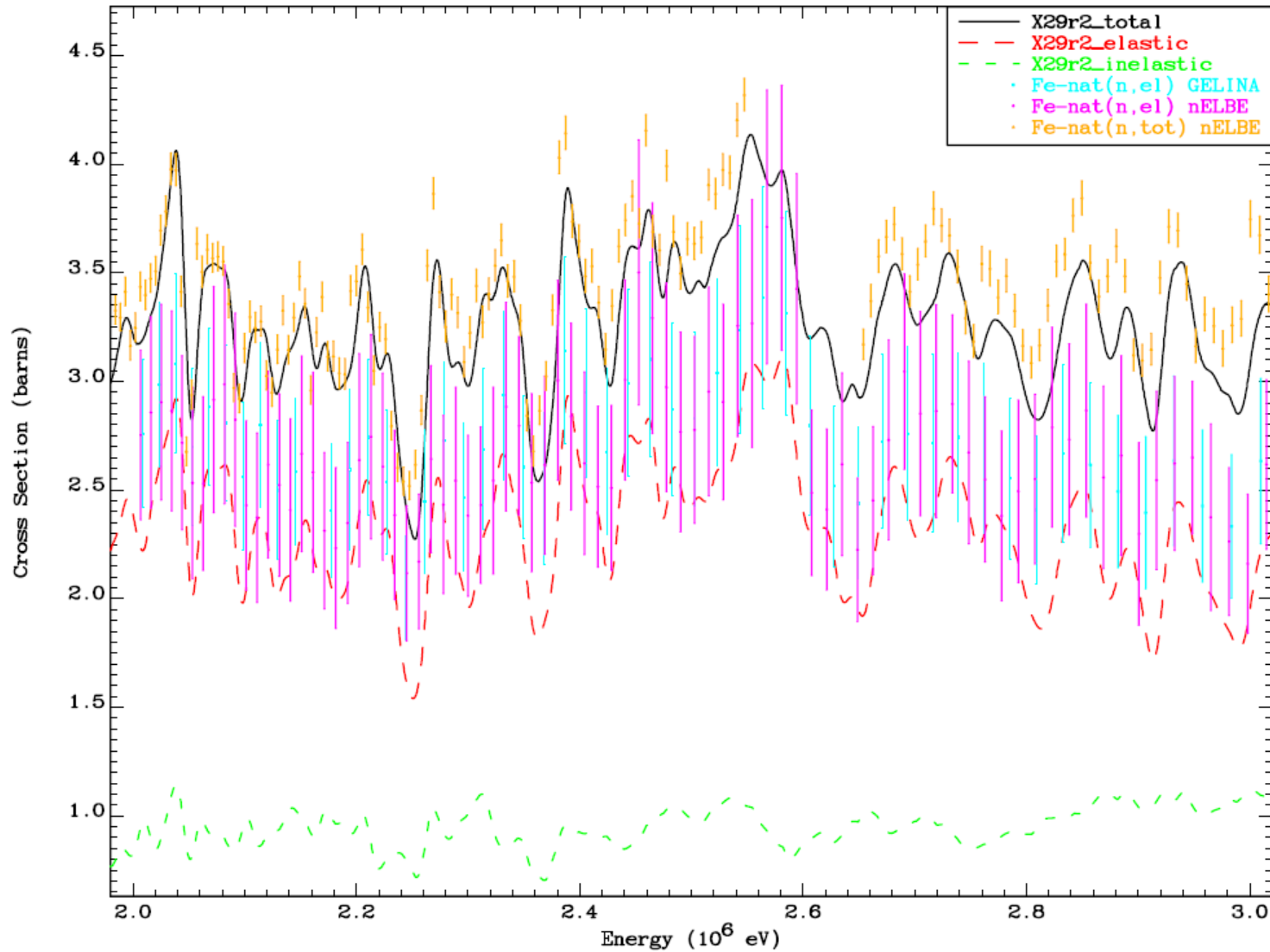
Differential experiments: σ_{inl}



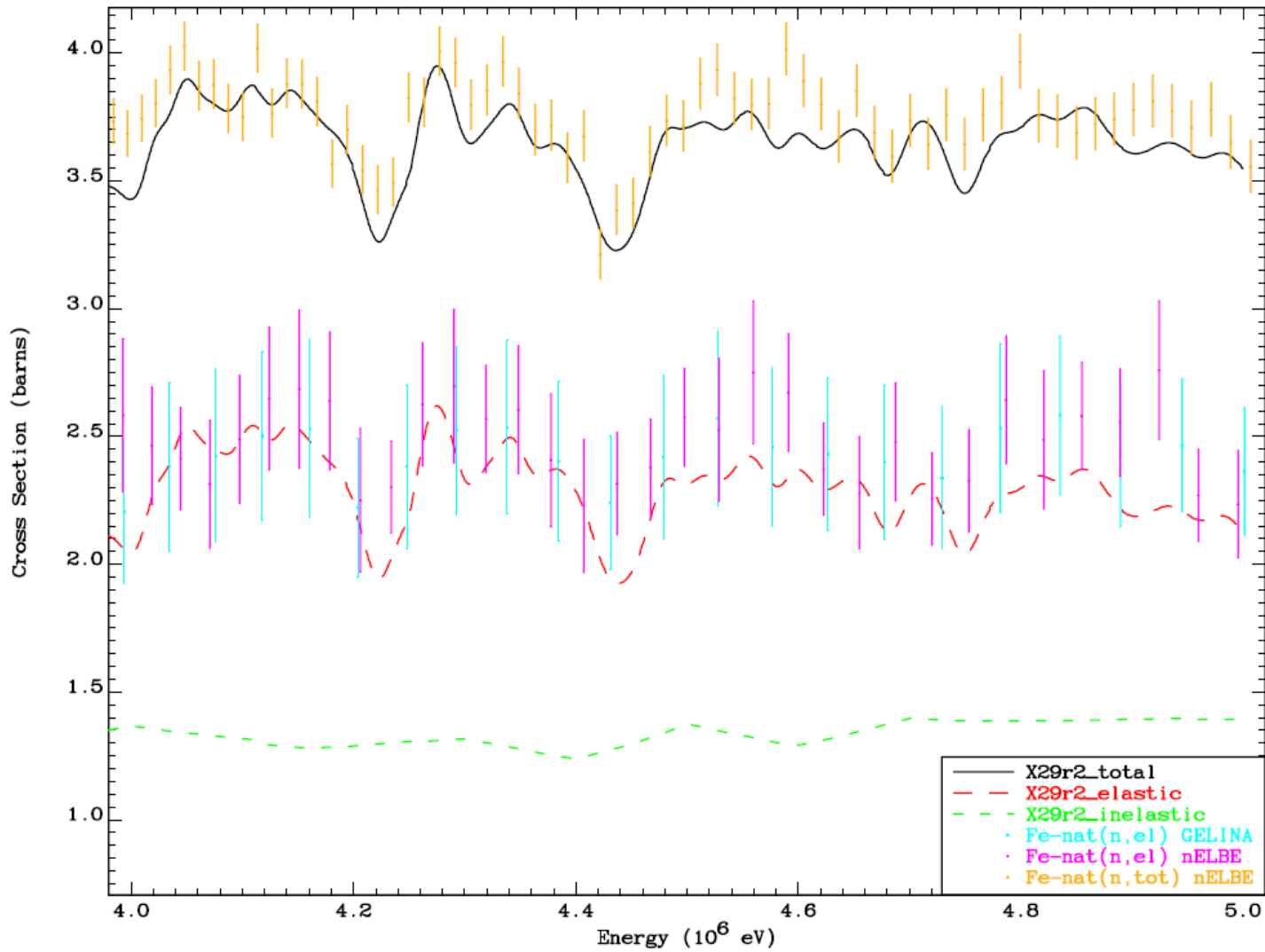
Differential experiments: σ_{inl}



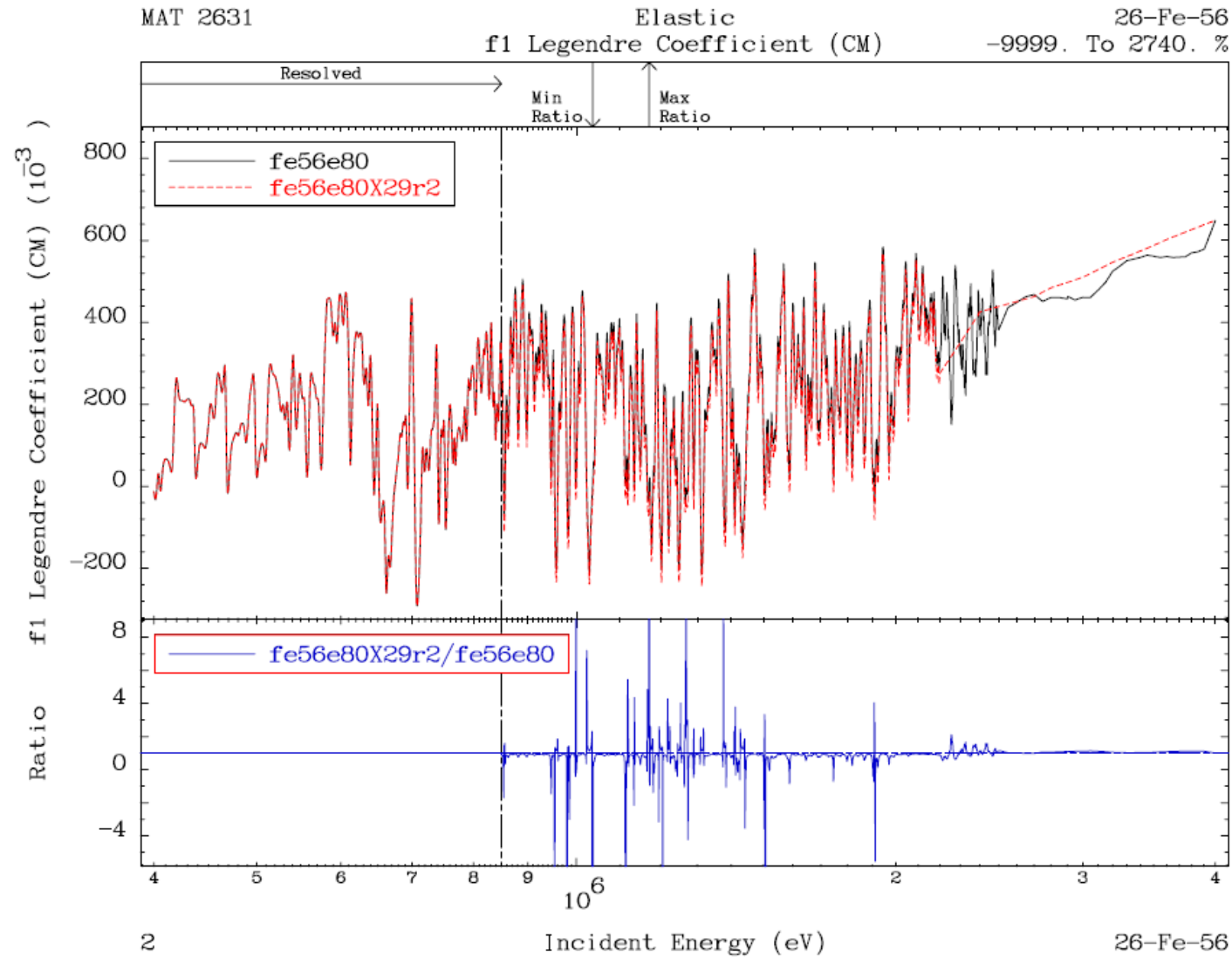
Differential experiments: σ_{tot} , σ_{el} , σ_{inl}



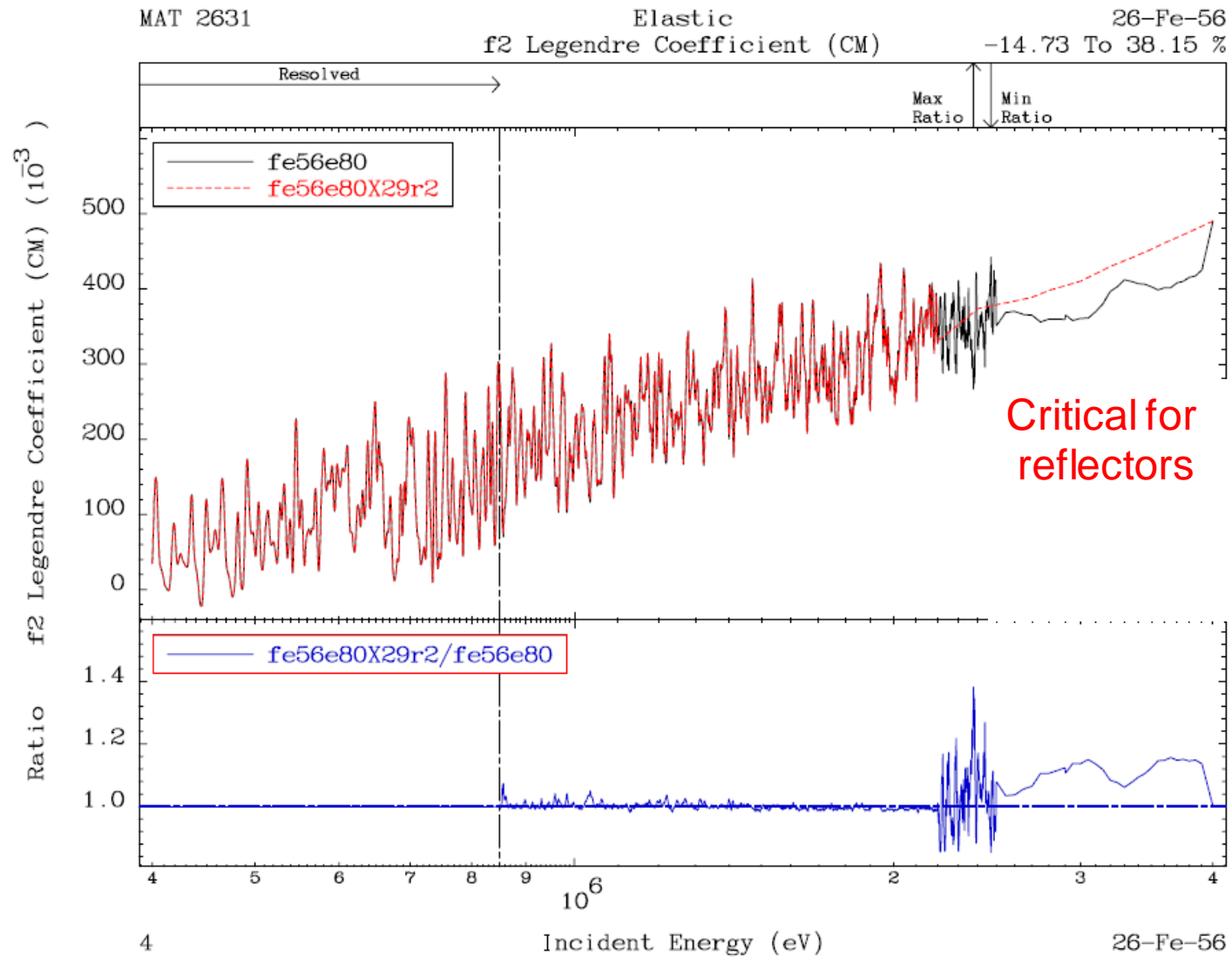
Differential experiments: σ_{tot} , σ_{el} , σ_{inl}



Fitted Kinney/Perey DA data



Fitted Kinney/Perey DA data



Performance of new ^{56}Fe file

- Independent analysis of IPPE benchmarks with a ^{252}Cf source from ICSBEP was made:
 - Problem with 60 cm diameter sphere with ^{252}Cf source is resolved.
 - Overestimation of the spectrum near 300 keV is significantly reduced.
- ICSBEP – IPPE broomstick experiments:
 - Flux attenuation in some energy regions in RRR in better agreement with measurements.

Useful benchmarks for ^{56}Fe file validation

1. IPPE leakage spectra from thick iron shells with a ^{252}Cf source (ICSBEP:ALARM-CF-FE-SHIELD-001)
2. ASPIS-Fe88 deep penetration case with a ^{235}U fast fission source (SINBAD)
3. IPPE leakage spectra from thick iron shells with a D-T source (SINBAD)
4. LLNL leakage spectra from thick iron shells with a D-T source
5. Oktavian leakage spectra from thick iron shells with a D-T source (SINBAD)

Useful benchmarks for ^{56}Fe file validation (cont.)



6. FNS-Fe thick slab ToF transmission spectra from a D-T source at different angles (SINBAD)
7. TIARA-Fe 40 MeV and 65 MeV transmission measurement (SINBAD)
8. IPPE iron broomstick experiments with quasi-monoenergetic p-T source (ICSBEP:FUND-IPPE-VDG-MULT-TRANS-001)

Less-useful benchmarks for ^{56}Fe file validation

- NIST-Fe leakage spectra from thick iron shells with a ^{252}Cf source (Stanka et al. NSE 134, 68-76 (2000)); coarser binning, but on average the results from IPPE iron spheres are confirmed
- Illinois-Fe leakage spectra from thick iron shells with a ^{252}Cf source (SINBAD); coarse
- EURACOS-Fe deep penetration case with a ^{235}U fast fission source (SINBAD); poor source definition
- LSD-RPI lead-slowing-down low-resolution cross section measurement (poor statistics)

Potentially-useful benchmarks for ^{56}Fe file validation

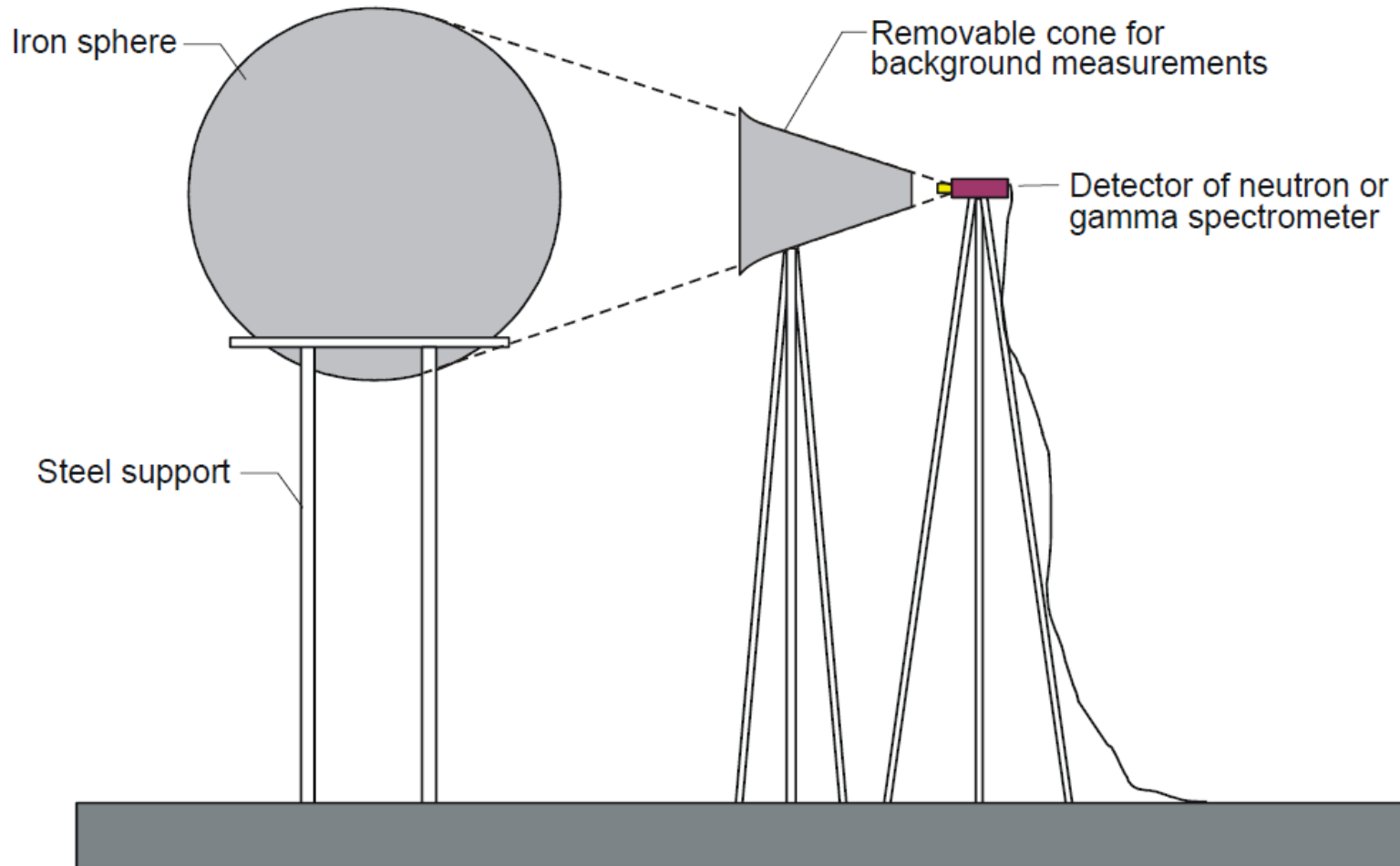
- KfK-Fe leakage spectra from thick iron shells with a ^{252}Cf source (SINBAD); (analysis by Simakov shows some contradiction with IPPE benchmark, MCNP input not available)
- NRI & Skoda leakage spectra from thick iron shells with a ^{252}Cf source, ANE 20,9, (1993), Sajo et al.; (new measurements from Rez also exist, but neither the measured data nor the MCNP model are available)
- ORNL Broomstick experiments (SINBAD) (not analysed)
- Ohio University – several benchmarks – e.g. Wenner et al. NSE 170 207 (2012); (details not available)
- RPI-Fe quasi-differential cross section measurement (waiting for data to be released)

1. IPPE spheres with ^{252}Cf source



- Benchmarks are available in ICSBEP for six spheres of diameters 20, 30, 40, 50, 60, 70cm

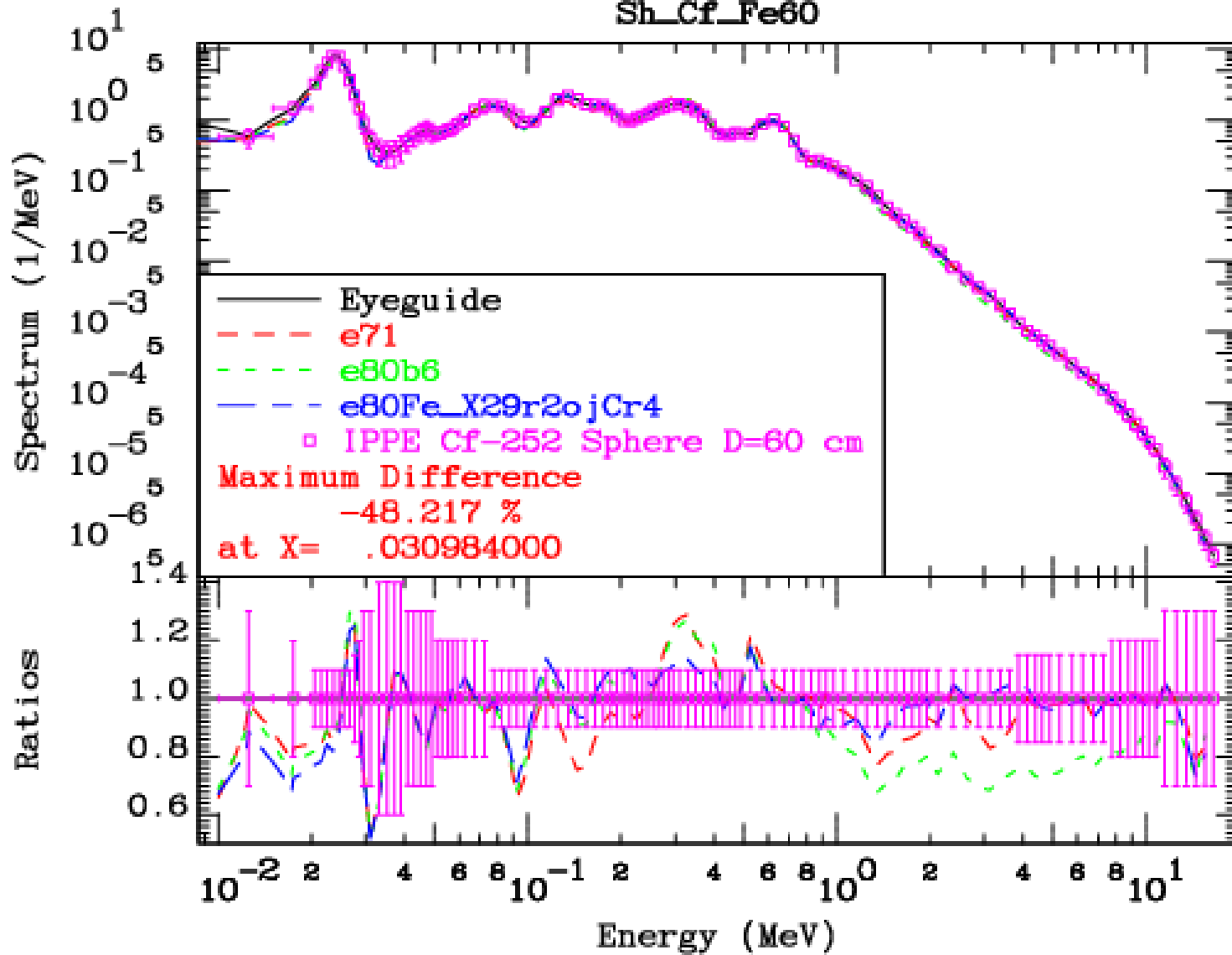
IPPE spheres with ^{252}Cf source



Drawing not to scale
Dimensions in cm

06-GA50000-234-2

IPPE Sphere Leakage Spectrum Sh_Cf_Fe60



Rez neutron leakage of $^{252}\text{Cf}(\text{sf})$ source, $\varnothing=100\text{cm}$ using Fe-56 evaluations

Tab.1 Assembly FE DIA100, R53; 200gpd, integral values, C/E
(Jansky, ND 2013, New York, [1])

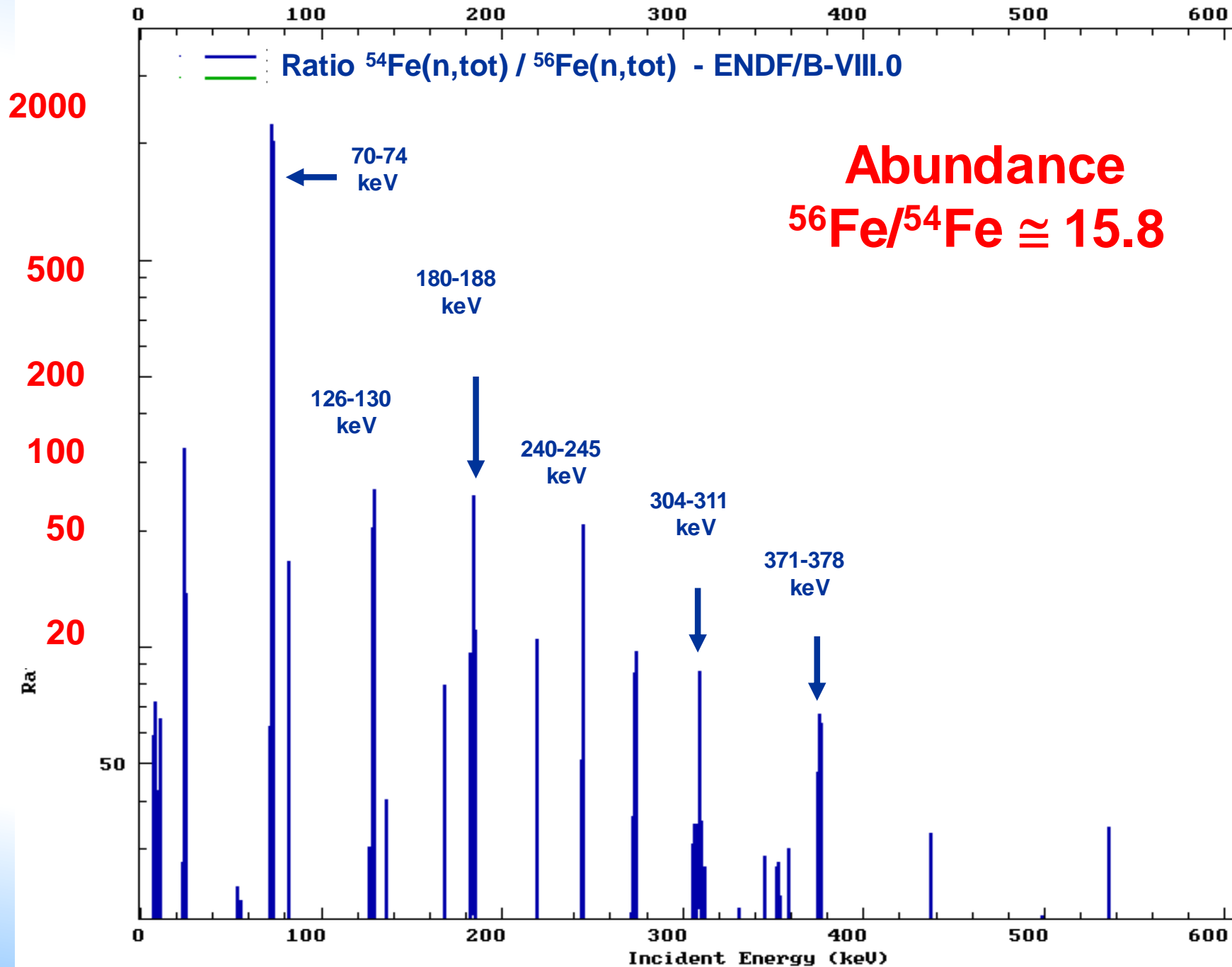
No.	En.range[MeV]		main peak [keV]	Library used for MCNP Calculation					
	from	to	in measurement	ENDF/B-VII.1	BROND-3	JENDL-4.0	JEFF-3.2T2	TENDL-2012	CENDL-3.1
0	0.013	1.290	total range	1.031	1.036	1.049	1.053	1.031	1.040
1	0.013	0.030	24.4	0.918	0.836	1.029	0.989	1.221	0.891
2	0.030	0.075		0.909	0.835	0.903	0.967	0.858	1.146
3	0.075	0.090	82	1.008	0.912	0.999	1.017	1.119	1.402
4	0.090	0.150	137	0.845	0.828	0.920	1.004	0.970	0.732
5	0.150	0.200	167+183	0.907	0.898	0.974	1.015	1.012	0.909
6	0.200	0.250		1.012	1.051	1.024	1.018	0.872	1.196
7	0.250	0.289	272	1.075	1.097	1.011	1.015	0.948	1.115
8	0.289	0.333	309	1.423	1.366	1.338	1.246	1.317	1.129
9	0.333	0.410	350	1.269	1.256	1.278	1.235	1.335	1.474
10	0.410	0.520		1.044	1.177	1.046	1.085	0.779	1.036
11	0.520	0.780	610+650+703	1.147	1.366	1.122	1.064	0.835	1.152
12	0.780	1.060		0.946	1.017	0.863	1.050	0.730	0.681
13	1.060	1.290		0.910	0.710	0.834	0.866	0.826	0.777

See next slide to compare energies

$^{54}\text{Fe}(\text{n,tot}) / ^{56}\text{Fe}(\text{n,tot})$

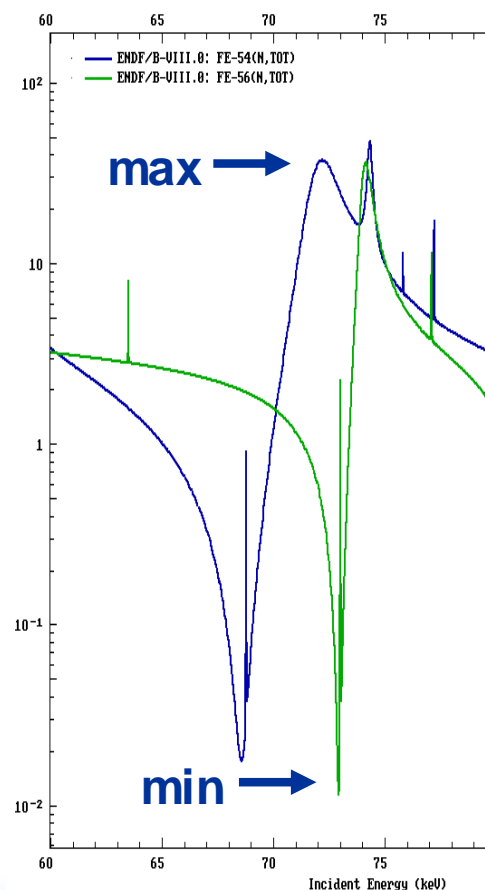
Jansky et al, JEFDOC 1218 (2018)
Presented at JEFF meeting held
in Madrid, Spain

Ratio $^{54}\text{Fe}(n,\text{tot}) / ^{56}\text{Fe}(n,\text{tot})$

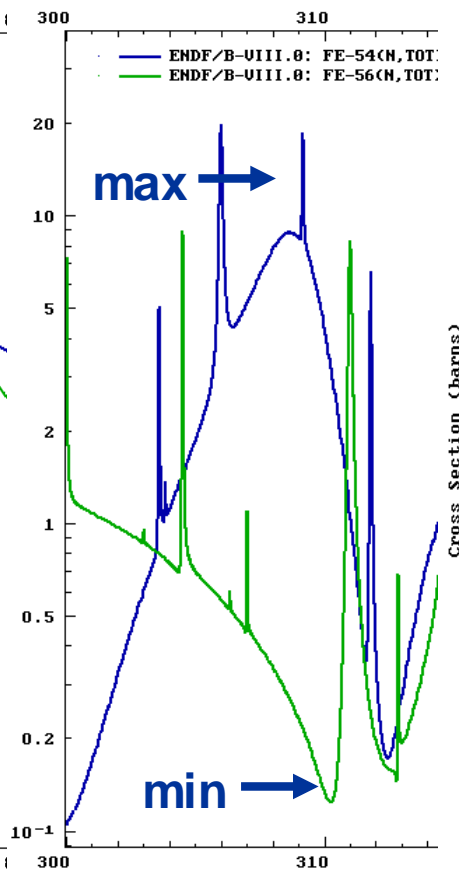




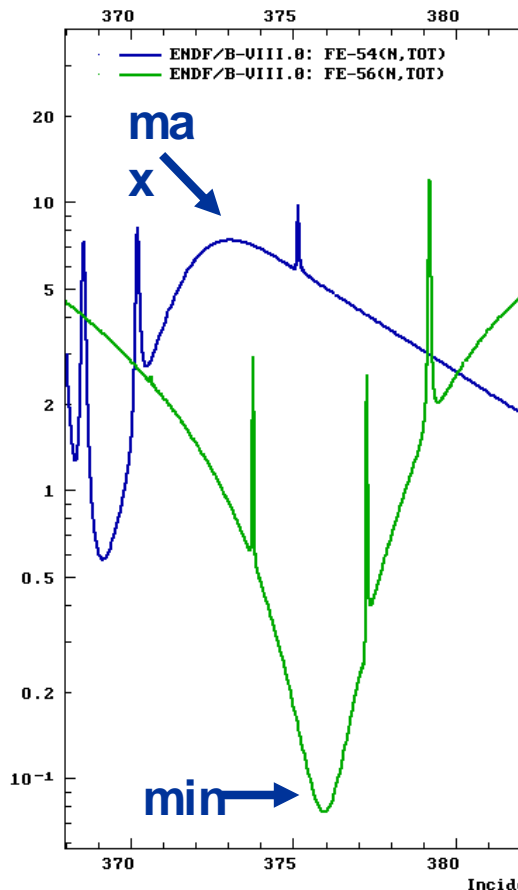
Importance of $^{56}\text{Fe}(n,\text{tot})$ minima: $\text{max}(^{54}\text{Fe}(n,\text{tot}))$ coincident with $\text{min}(^{56}\text{Fe}(n,\text{tot}))$



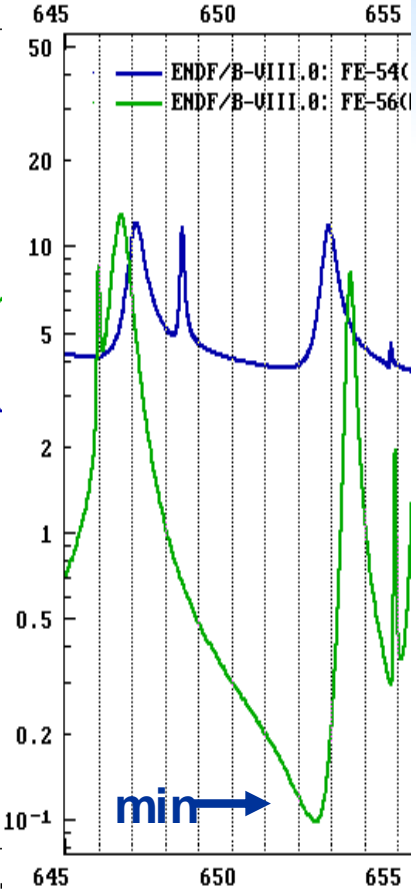
$E_n \approx 70-74$ keV



$E_n \approx 304-311$ keV



$E_n \approx 371-378$ keV



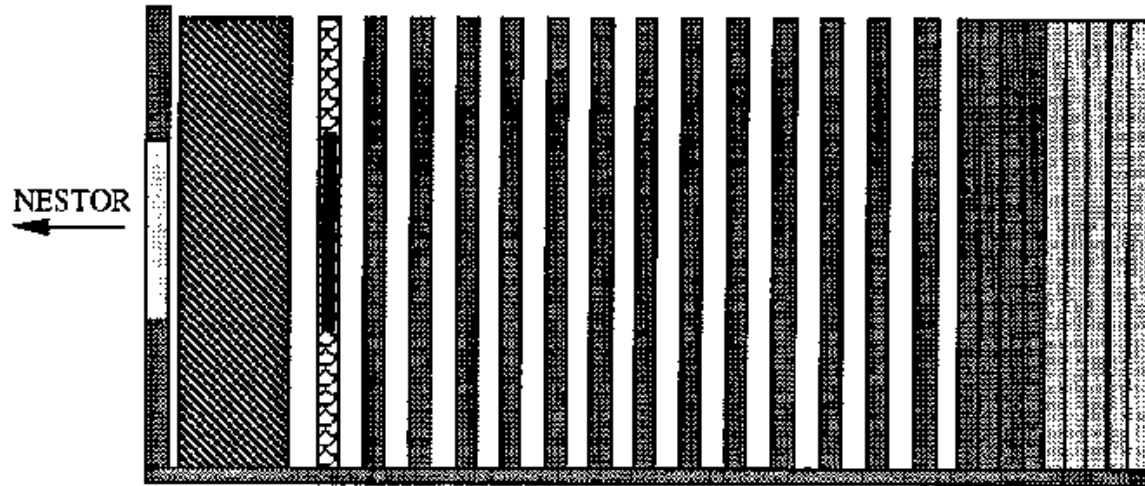
$E_n \approx 648-654$ keV

2. ASPIS-Fe-88 benchmark







- Available in SINBAD, no MCNP model
- Contract from IAEA with B. Kos, JSI (working with I. Kodeli)
- Input models with variance reduction delivered
- Agreement with measured activities are generally good, except for $Al(n,a)$ systematic over-prediction – possible Na impurity?

ASPIS-Fe-88 benchmark (cont.)

Figure 1 Schematic side elevation of the shield in the iron 88 single material benchmark experiment

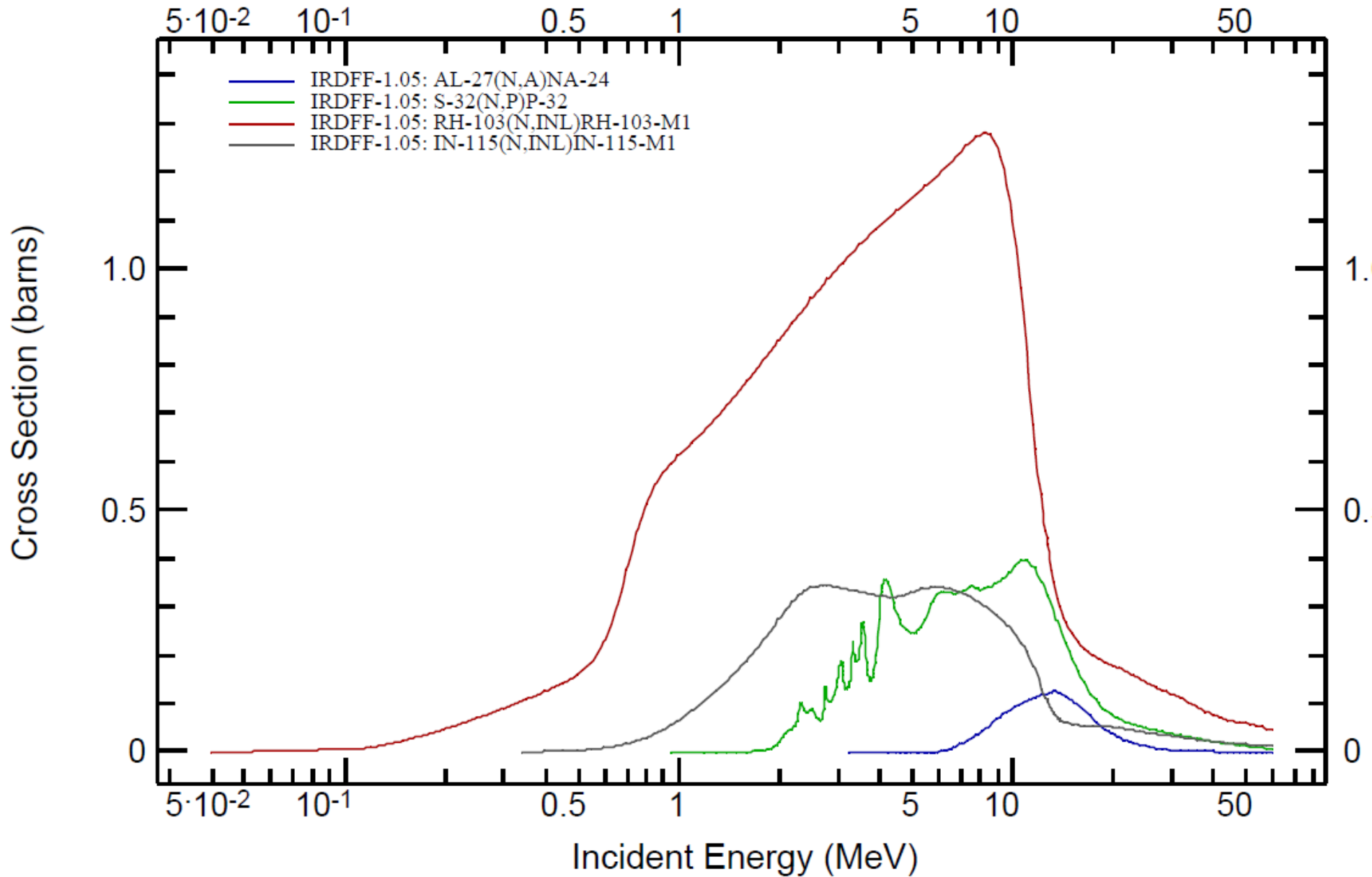


KEY

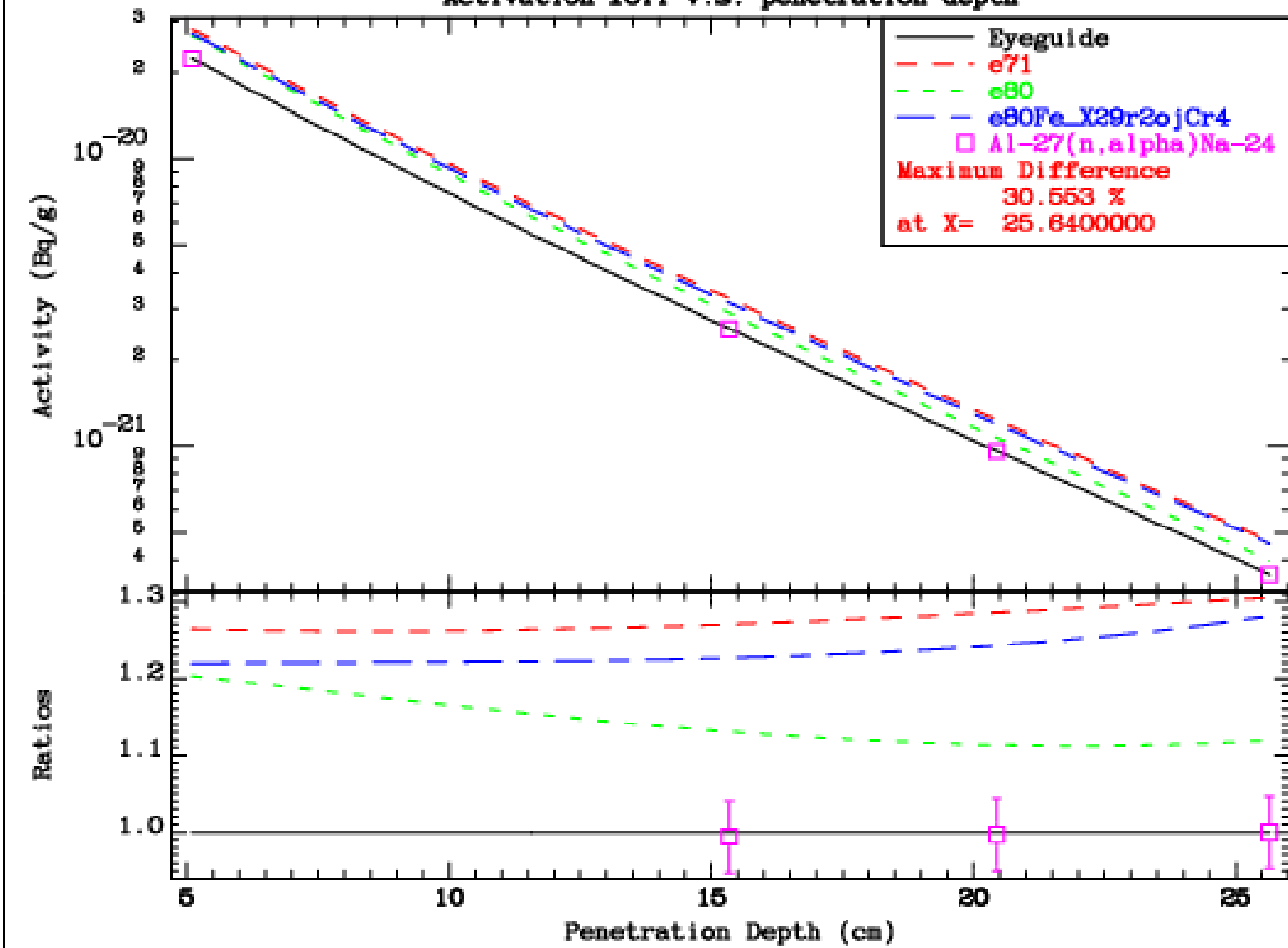
-  Fuel
-  Mild Steel
-  Stainless Steel
-  Fission Plate
-  Graphite
-  Aluminium

All components are 182.9cm wide by 191.0cm high

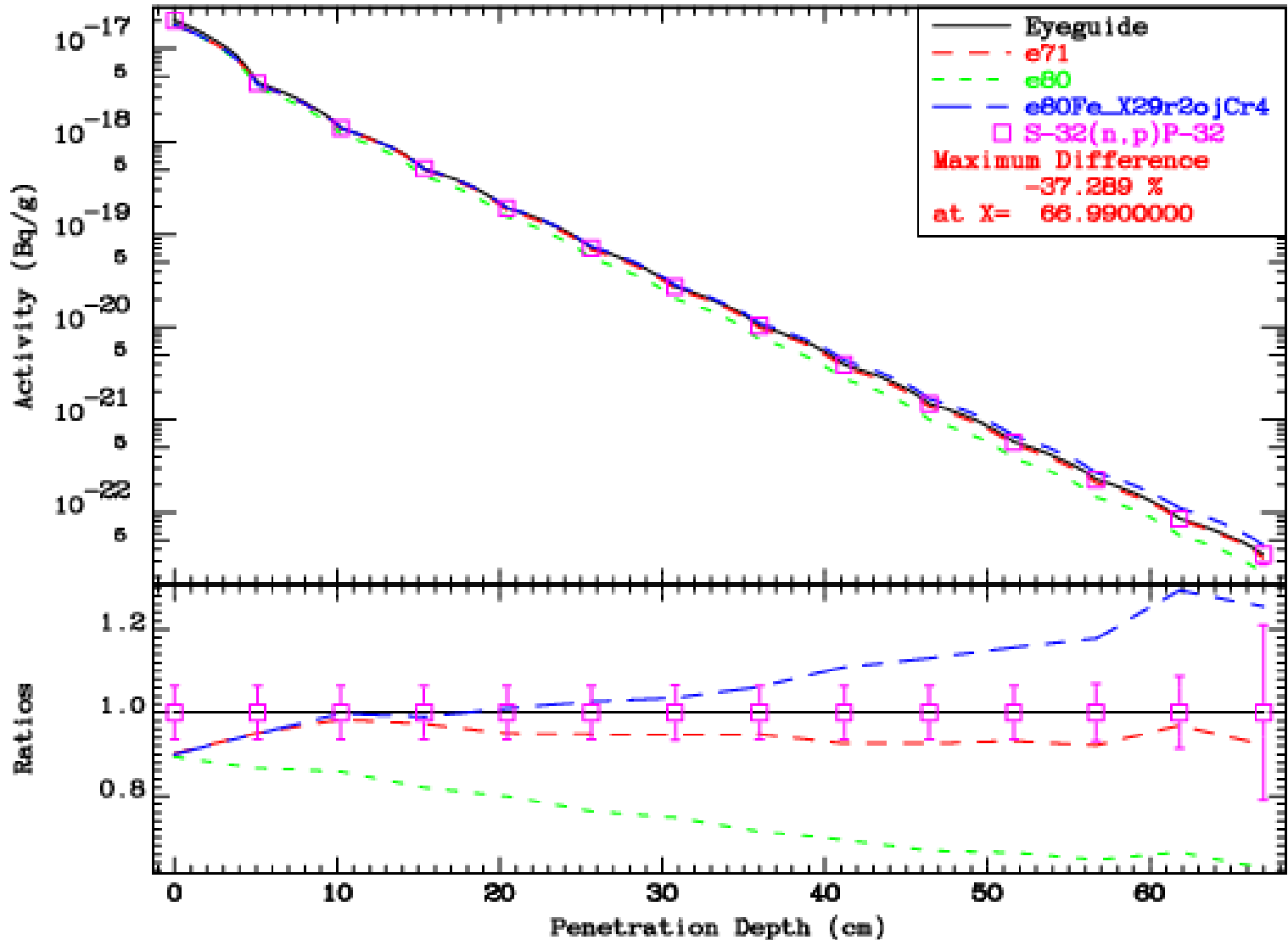
Not To Scale



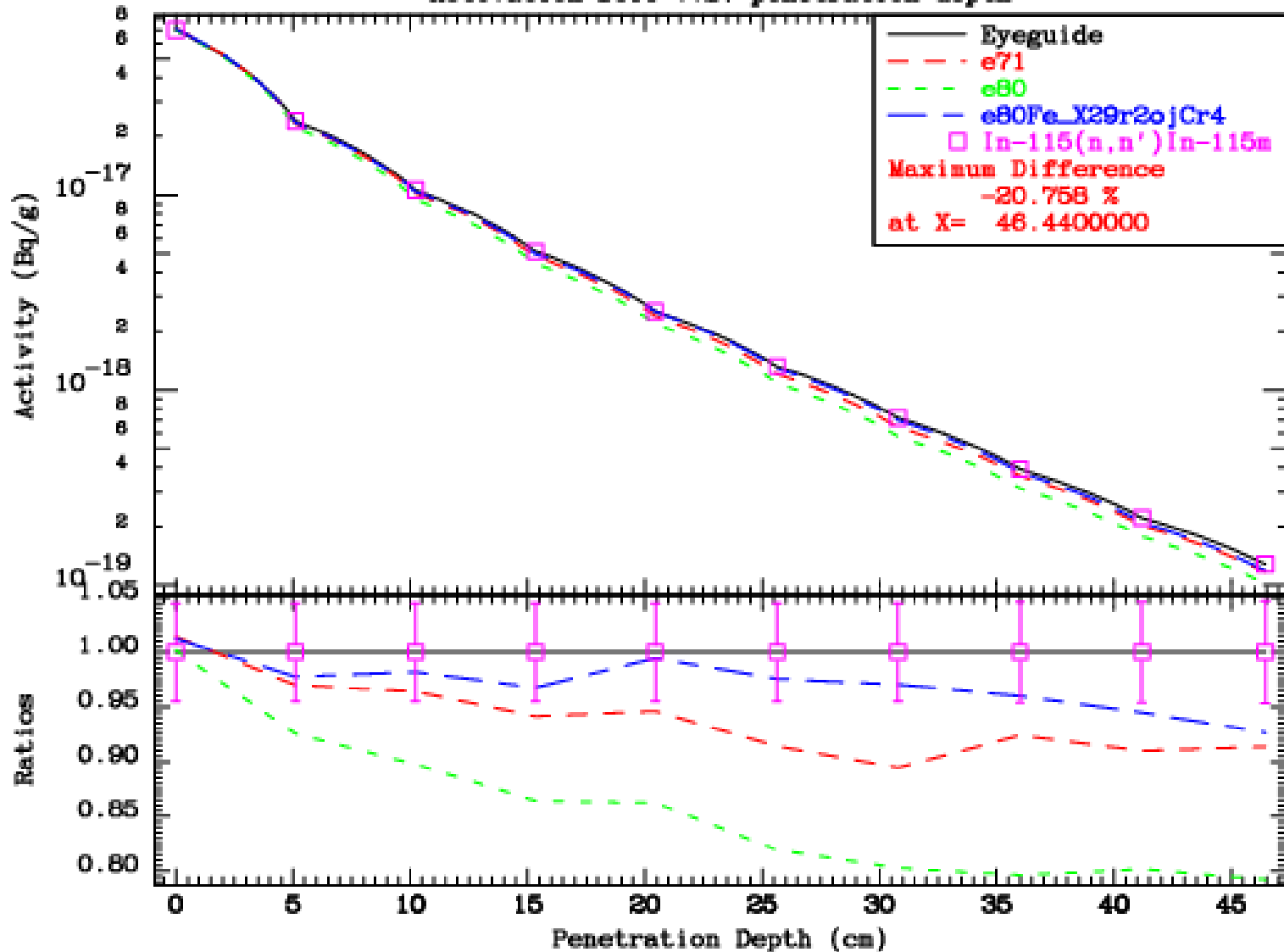
Benchmark aspis-fe88_al
 Activation foil v.s. penetration depth



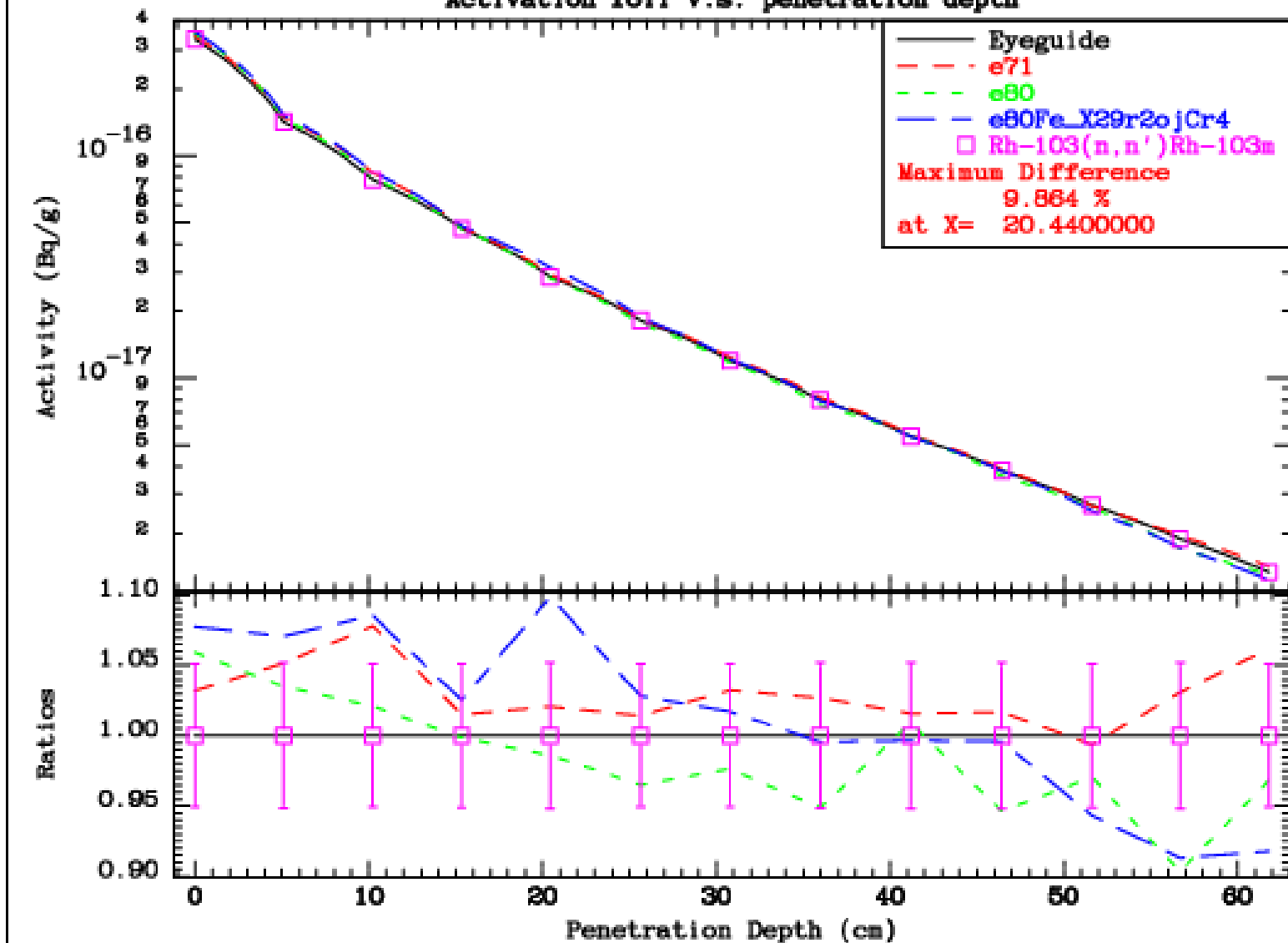
Benchmark aspis-fe88_s
 Activation foil v.s. penetration depth



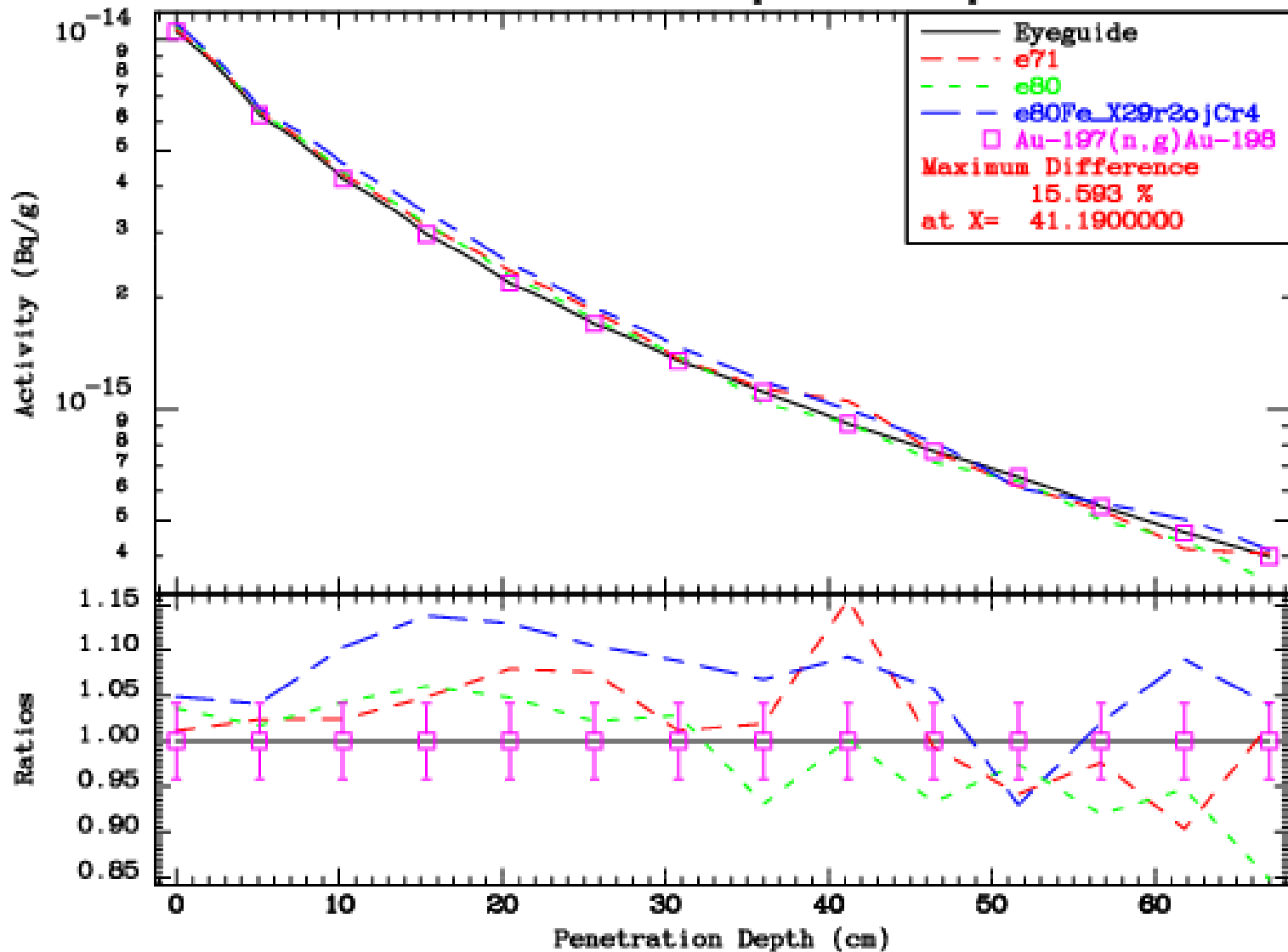
Benchmark aspis-fe88_in
 Activation foil v.s. penetration depth



Benchmark aspis-fe88_rh
 Activation foil v.s. penetration depth



Benchmark aspis-fe88_au
 Activation foil v.s. penetration depth



3. IPPE spheres with D-T source

- Benchmarks are available in SINBAD but without adequate MCNP inputs
- Analysed previously by A. Milocco at JSI (working with A. Trkov and I. Kodeli), computational model in the time domain, converted to energy

IPPE spheres with D-T source (cont.)

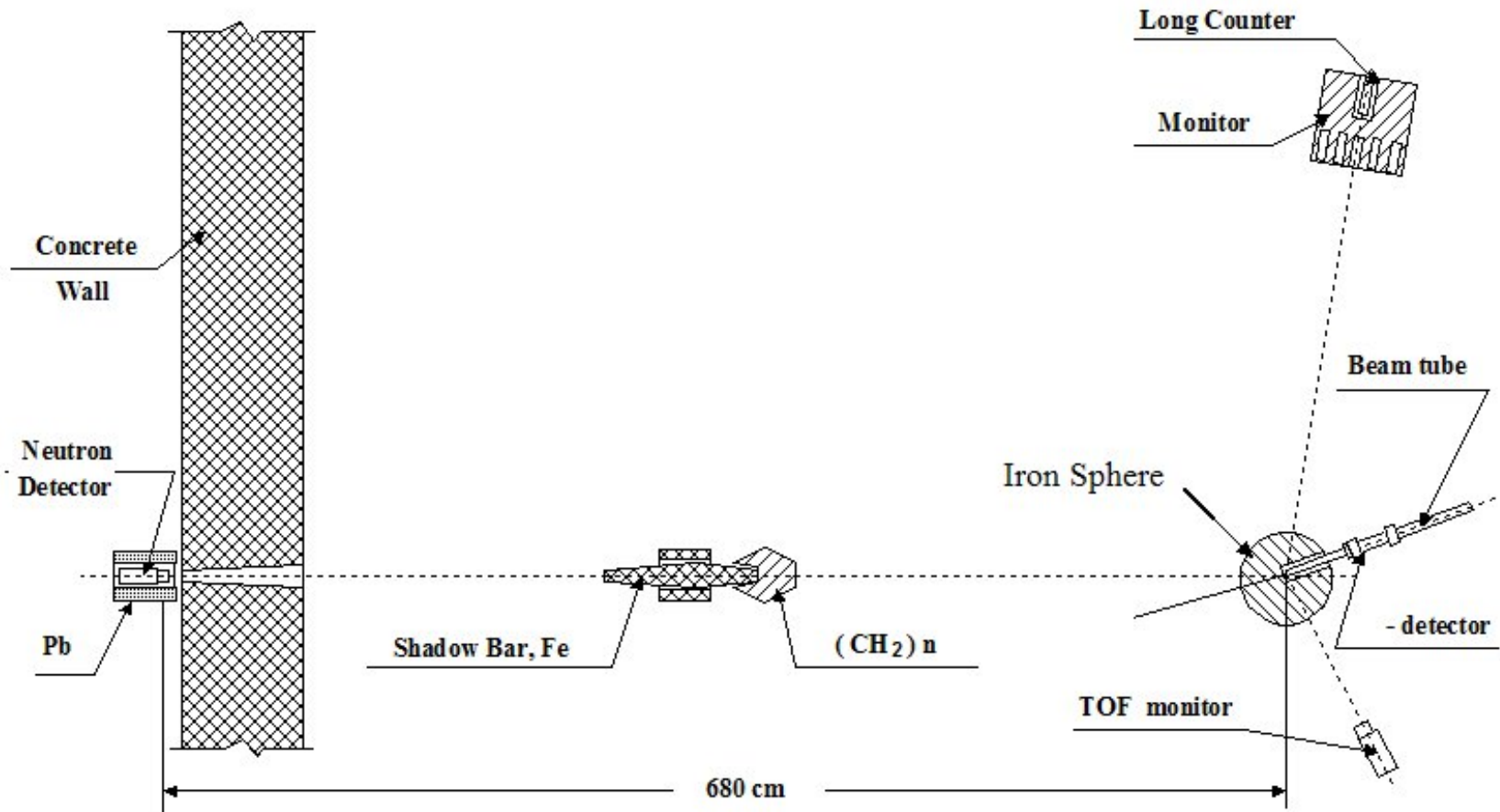
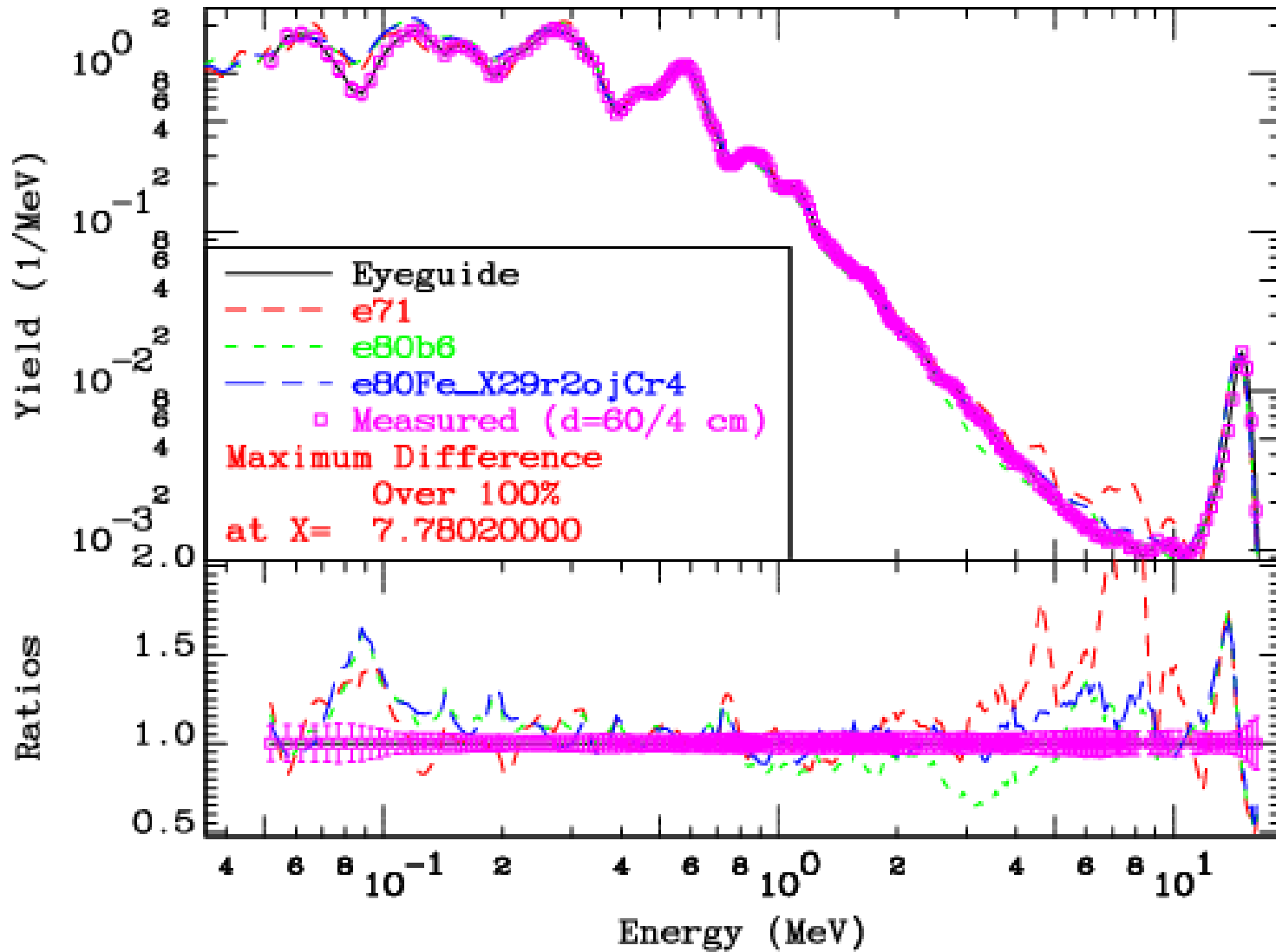


Fig. 1. Lay-out of experiment for measuring the neutron leakage spectra from iron spheres.

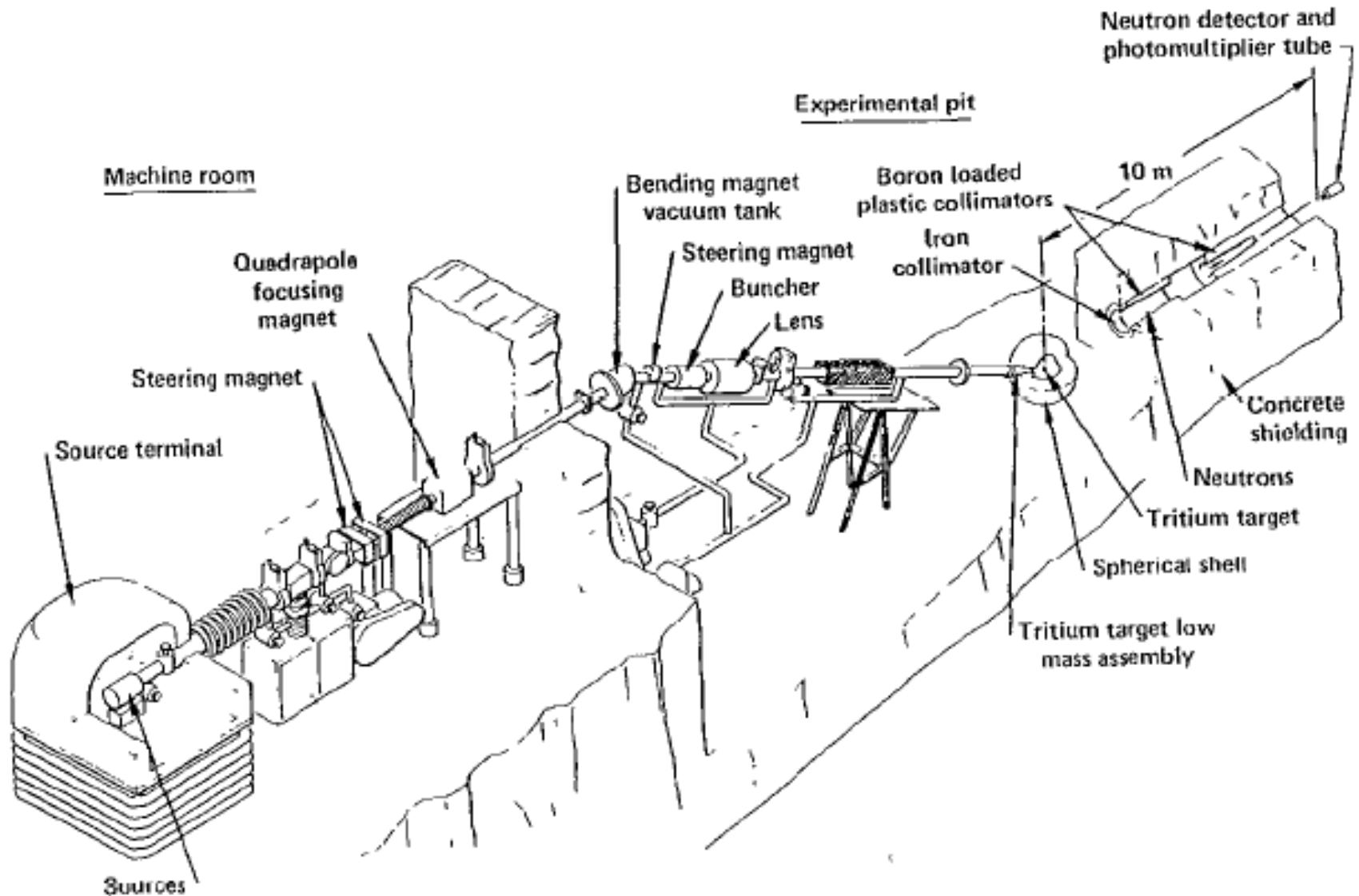
IPPE Fe Sphere Leakage Spectrum D-T Source
IPPE_Fe-5



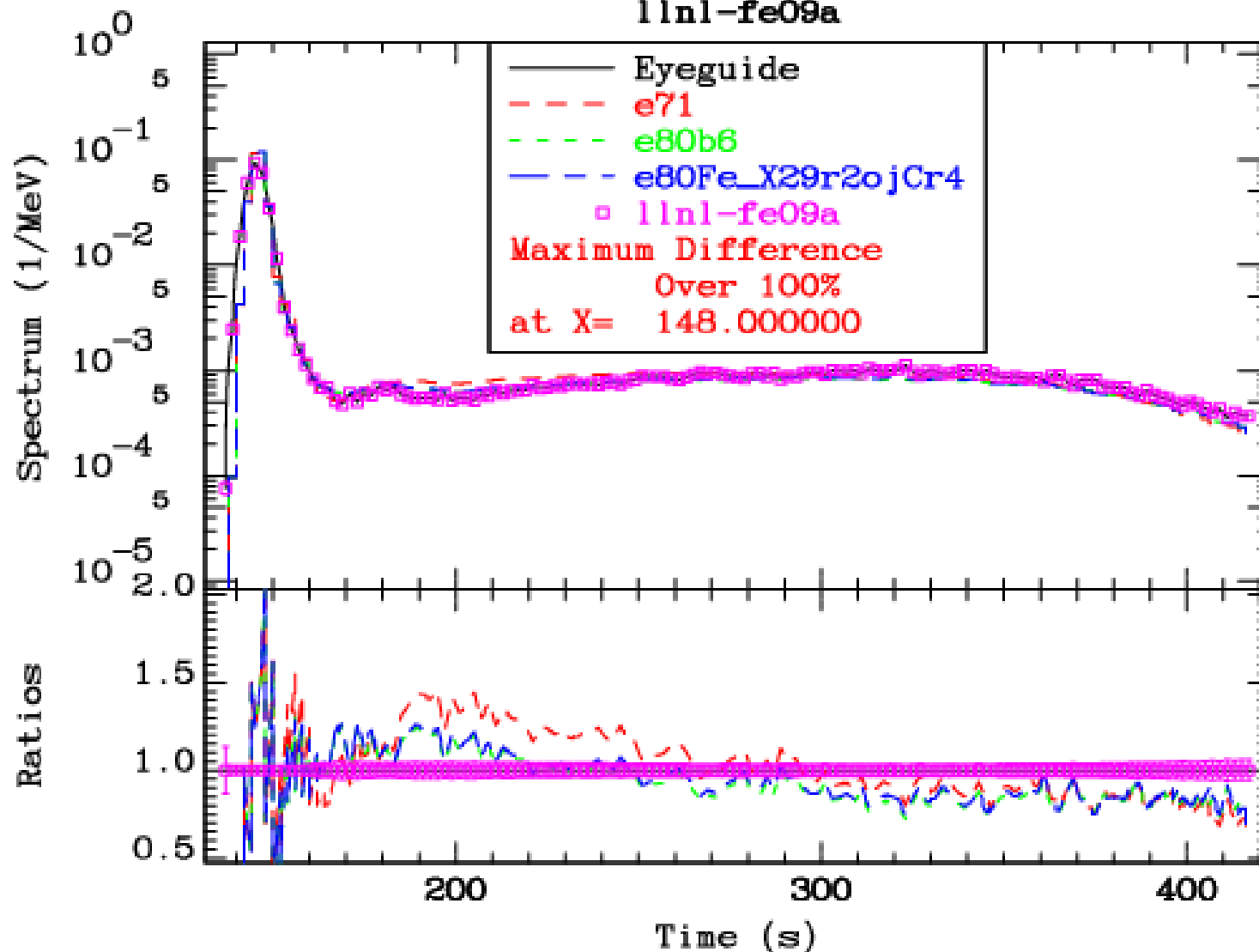
4. LLNL spheres with D-T source

- Experiments from Lawrence Livermore National Laboratory
- Two spheres 8.92 cm diam. (0.9 m.f.p.) and 44.6 cm diam. (4.8 m.f.p.) and two detectors
- Computational models by S. Frankle (obtained from LANL); computational model in the time domain, converted to energy.
- Similar to IPPE benchmark with D-T source, but over a shorter energy range – supports the observation of a difference in gradient (difference is smaller with the new file)

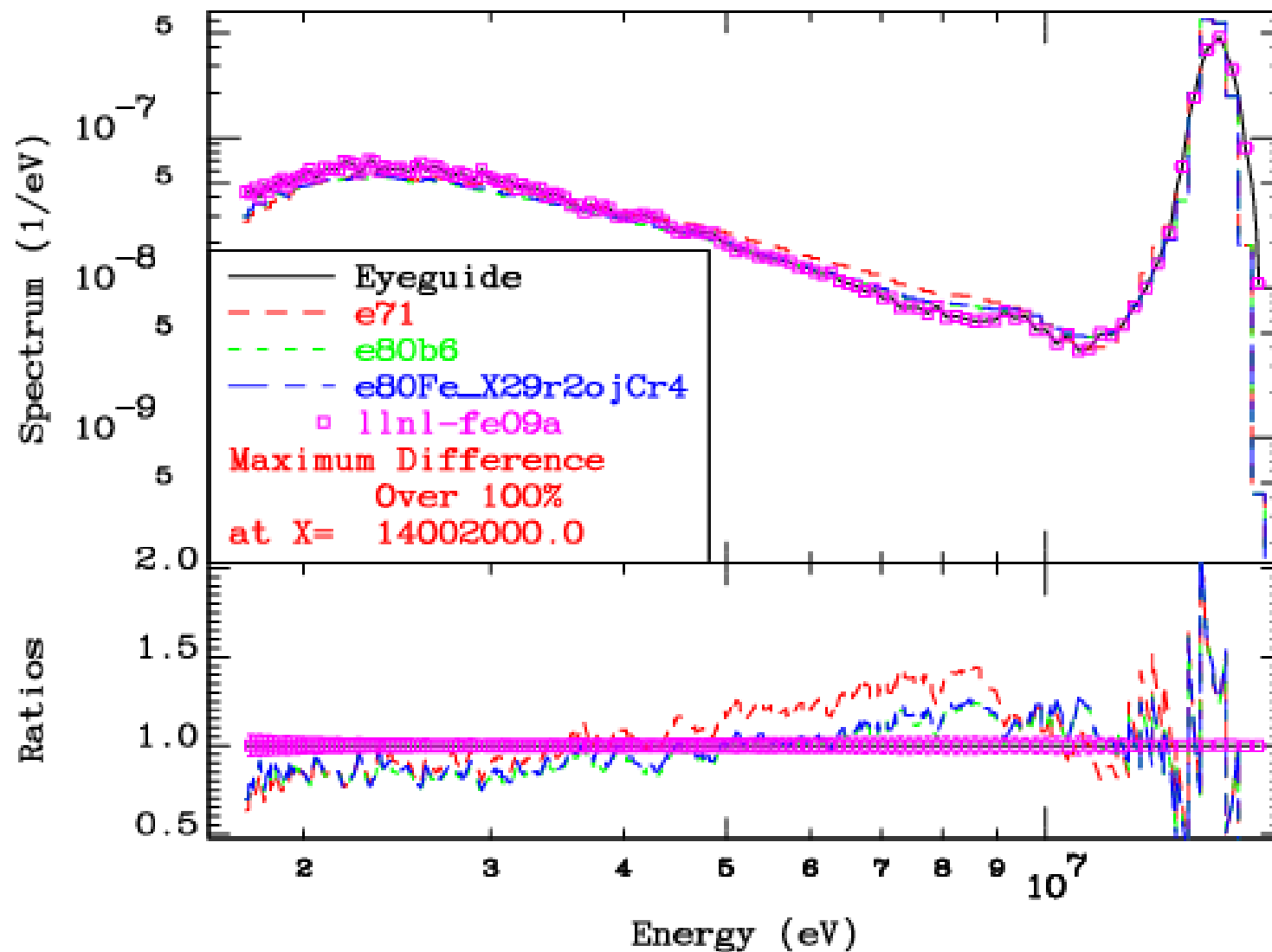
LLNL spheres with D-T source (cont.)



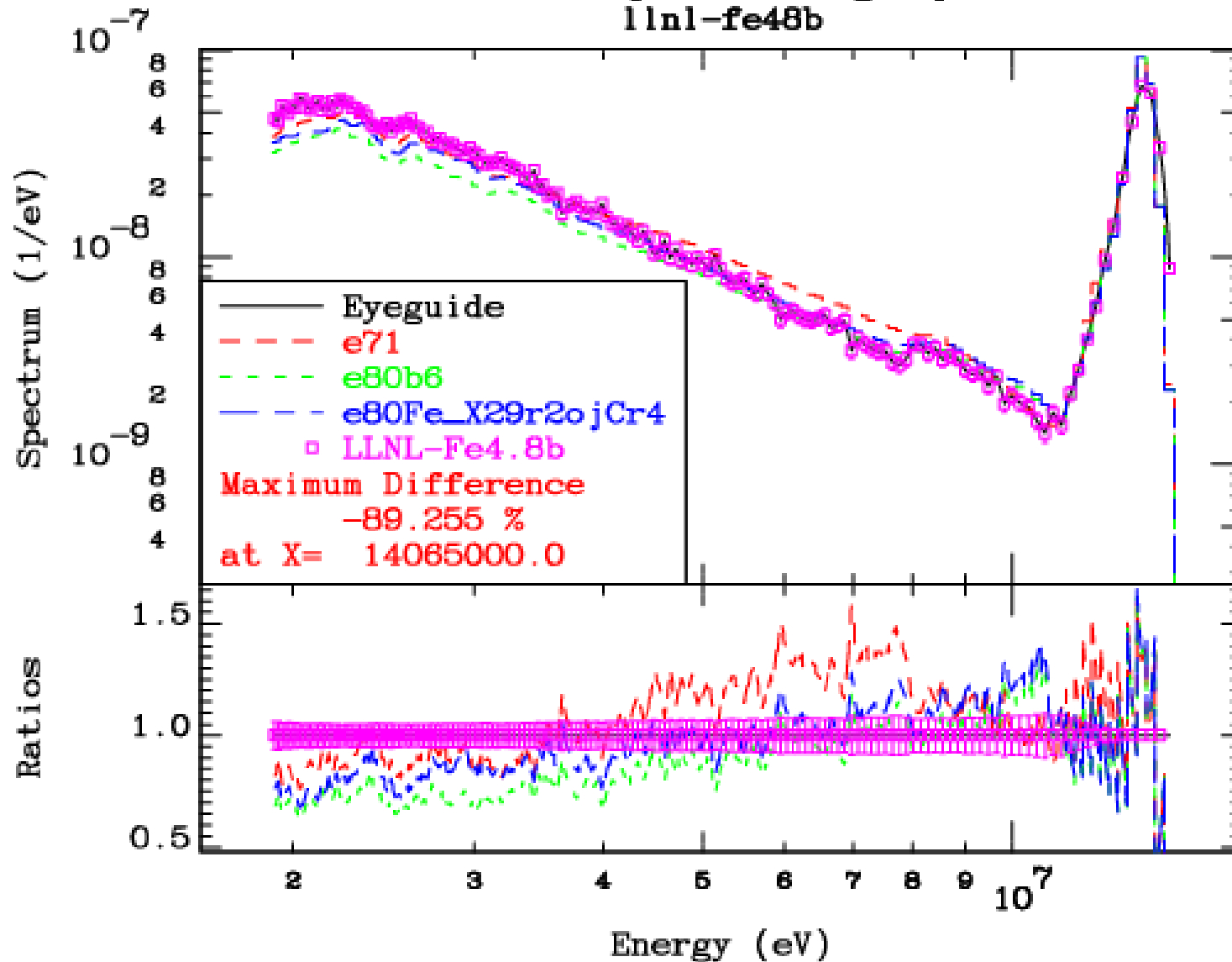
LLNL Pulsed Sphere Leakage Spectrum llnl-fe09a



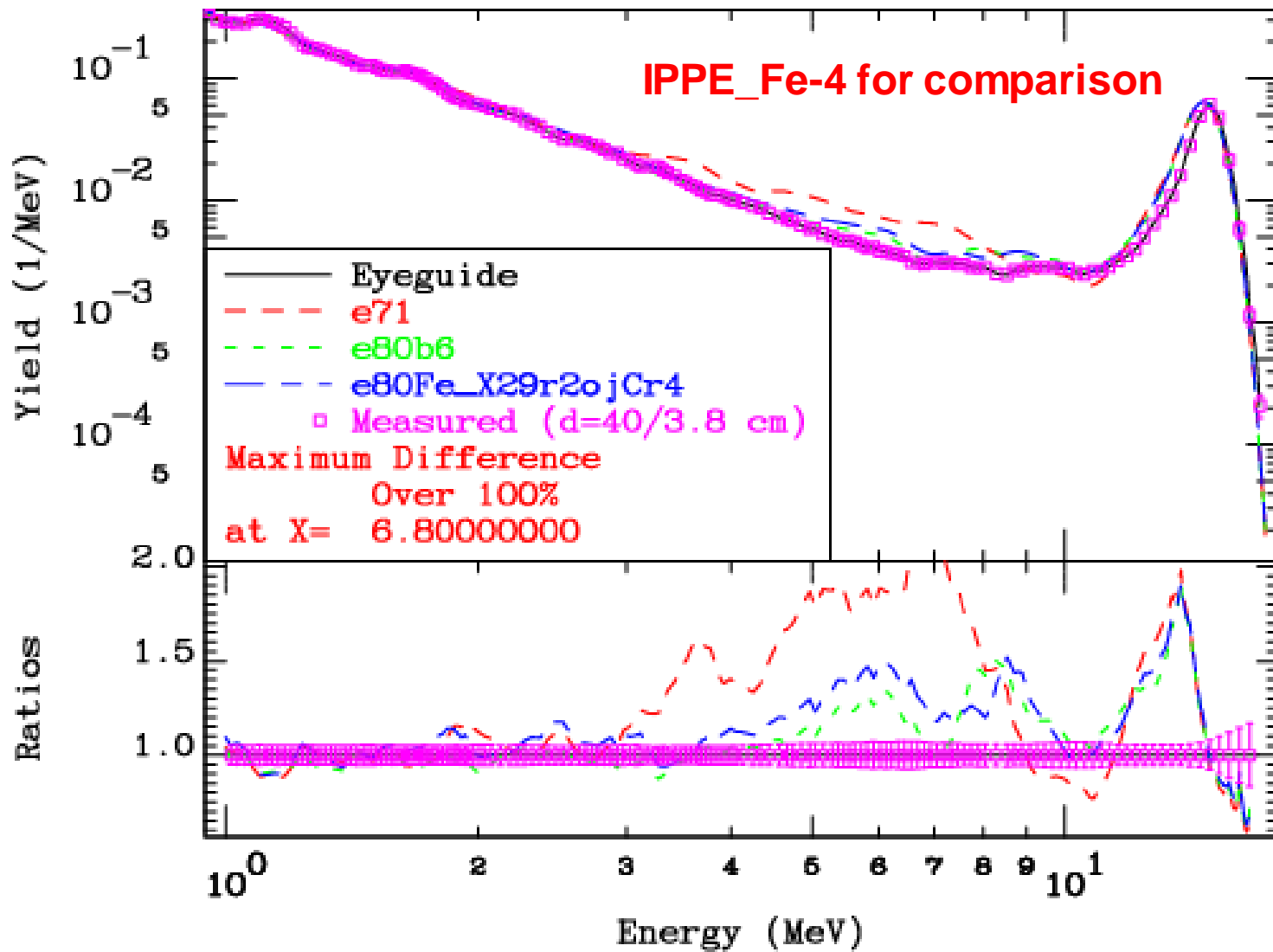
LLNL Pulsed Sphere Leakage Spectrum llnl-fe09a



LLNL Pulsed Sphere Leakage Spectrum llnl-fe48b



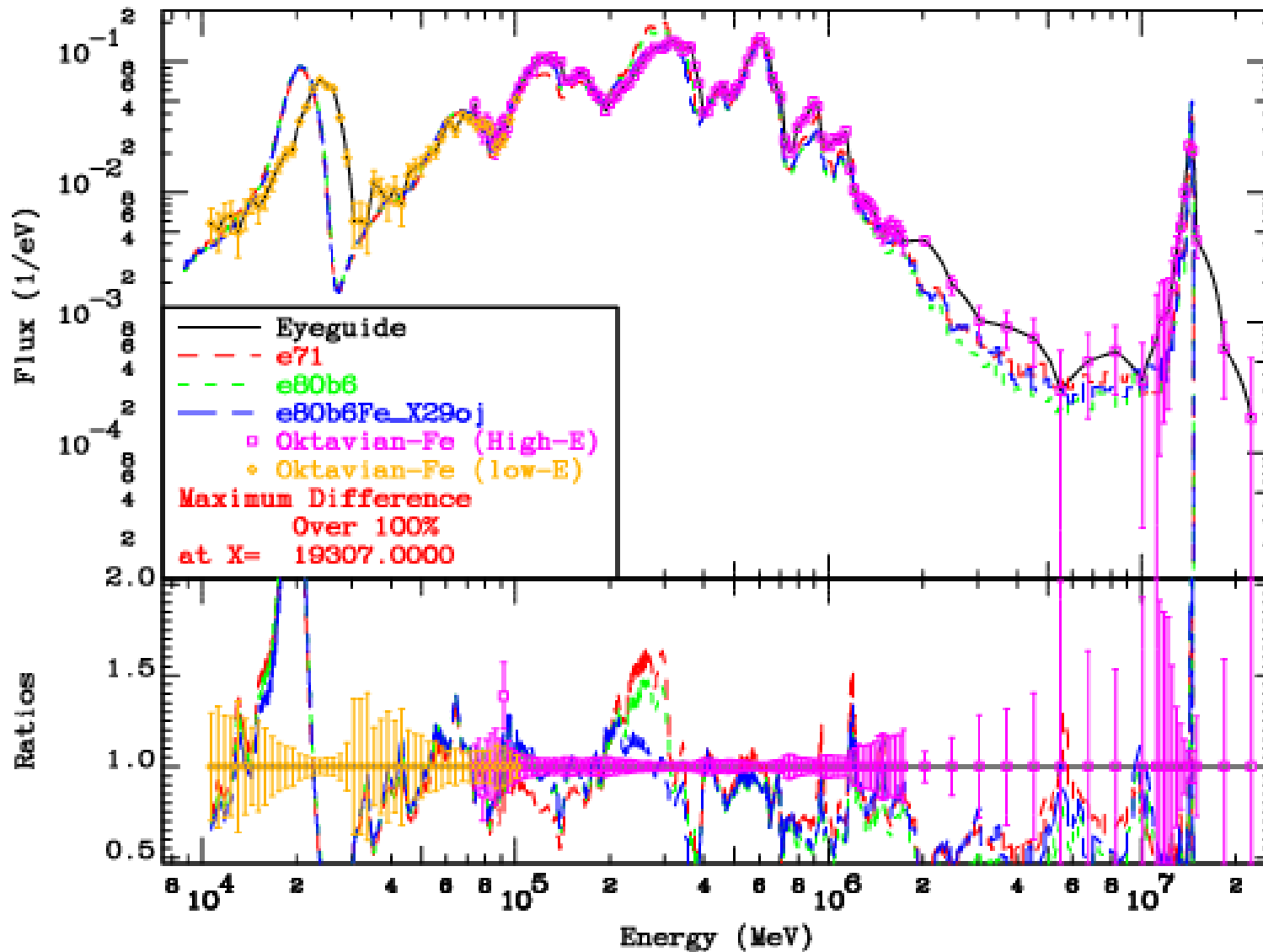
IPPE Fe Sphere Leakage Spectrum D-T Source
IPPE_Fe-4



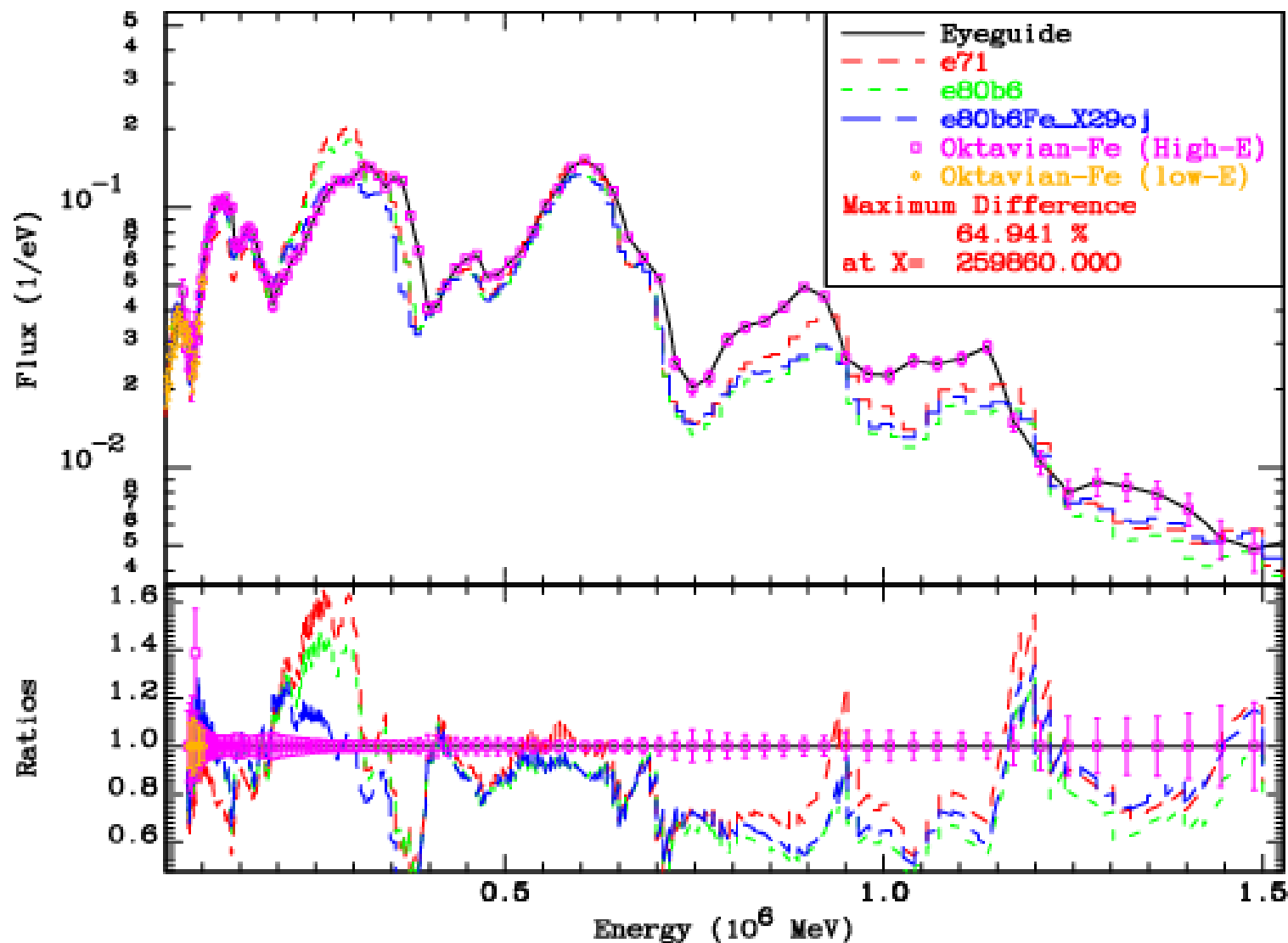
5. Oktavian-Fe sphere with D-T source

- Experiments from Osaka University documented in SINBAD
- Fe sphere of 100.64 cm diameter
- At energies above 0.7 MeV significant deviations from measured values are observed
- Above 2 MeV the measurements are not reliable
- Low-energy measurement seems to be shifted in energy

Oktavian sphere 1 m Leakage spectrum
D-T 14 MeV Source



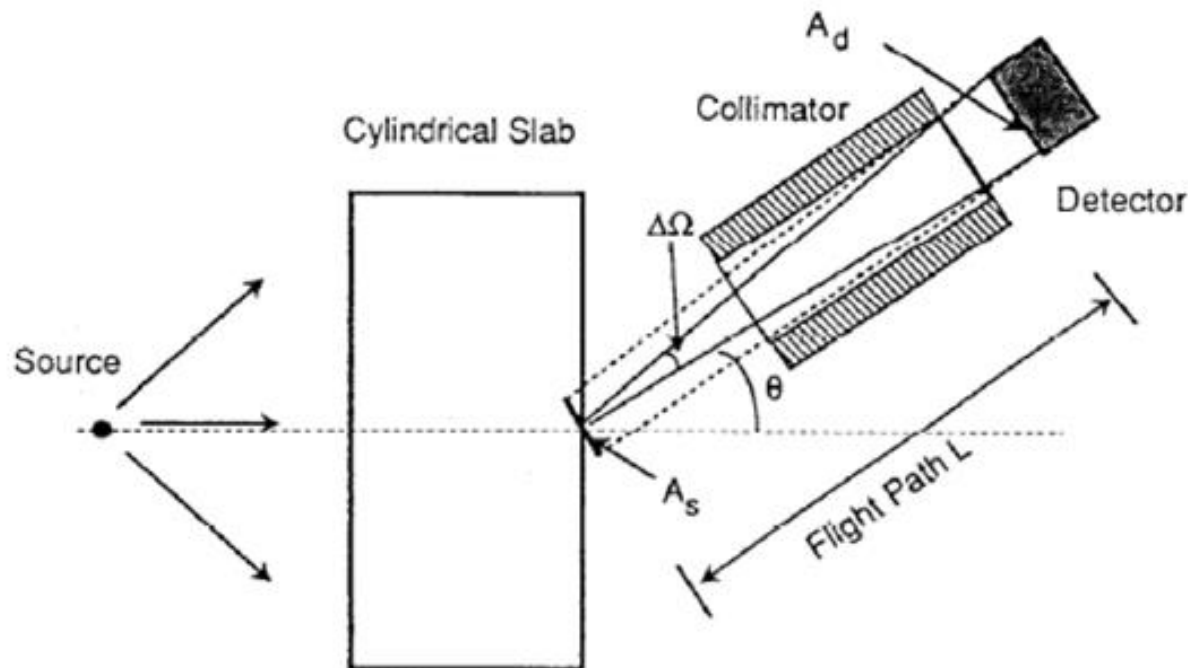
Oktavian sphere 1 m Leakage spectrum
D-T 14 MeV Source



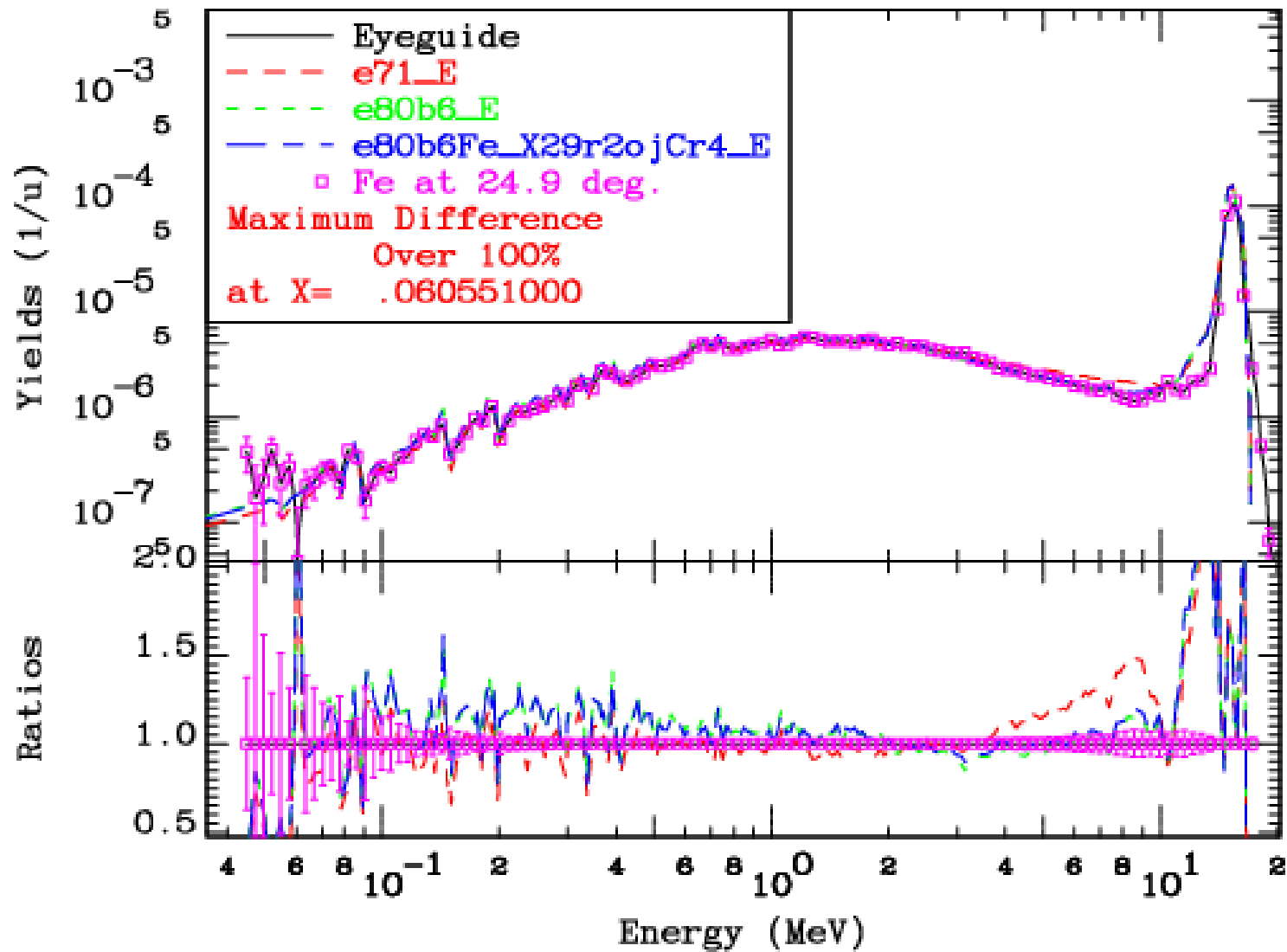
6. FNS-Fe thick slab transmission spectra at different angles

- Recent re-analysis by B. Kos from JSI with weight-windows variance reduction

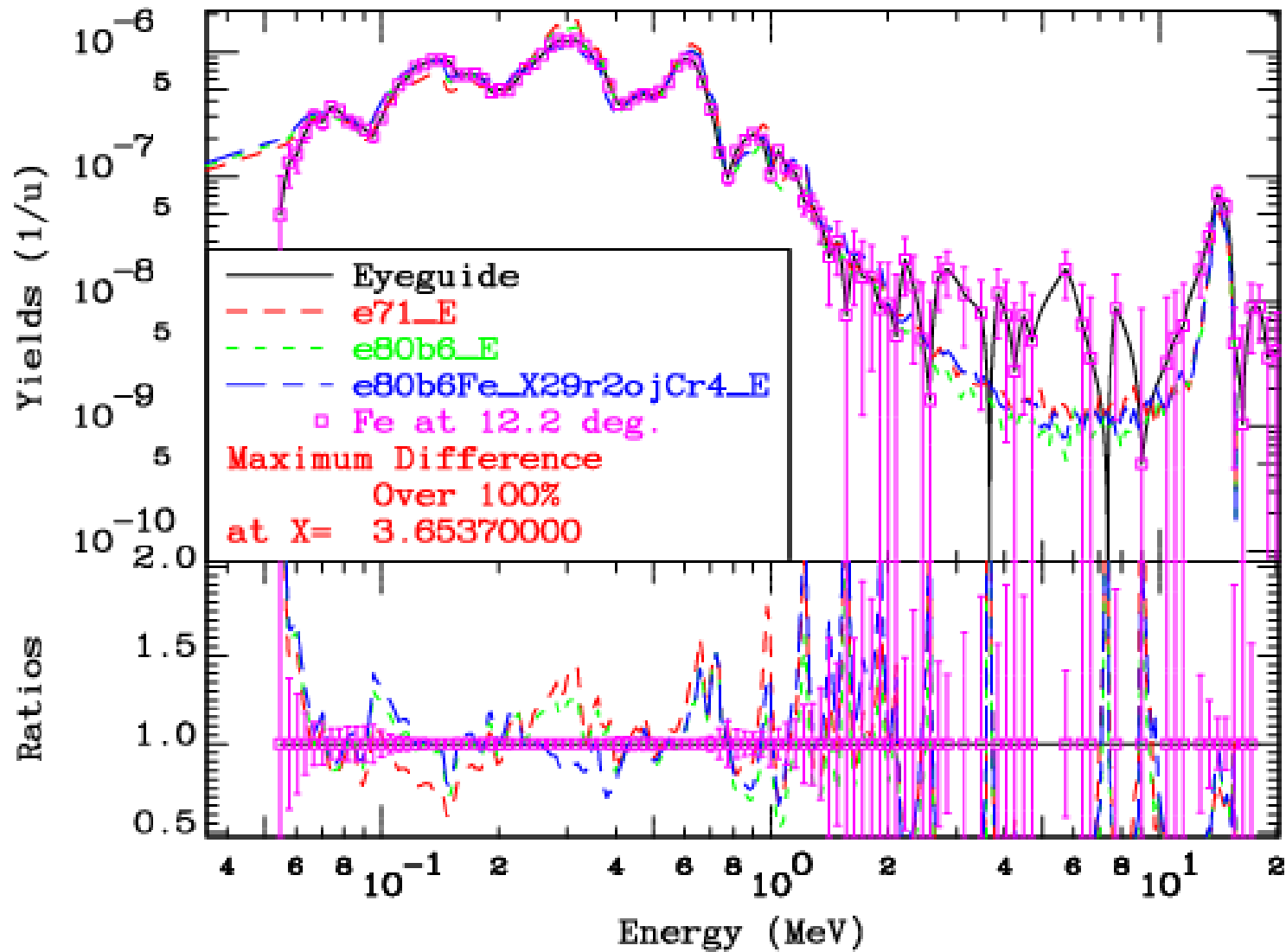
1. TOF



FNS-Fe Leakage Spectrum D-T Source
Fe_500_050_FNS_TOF 24.9 degrees



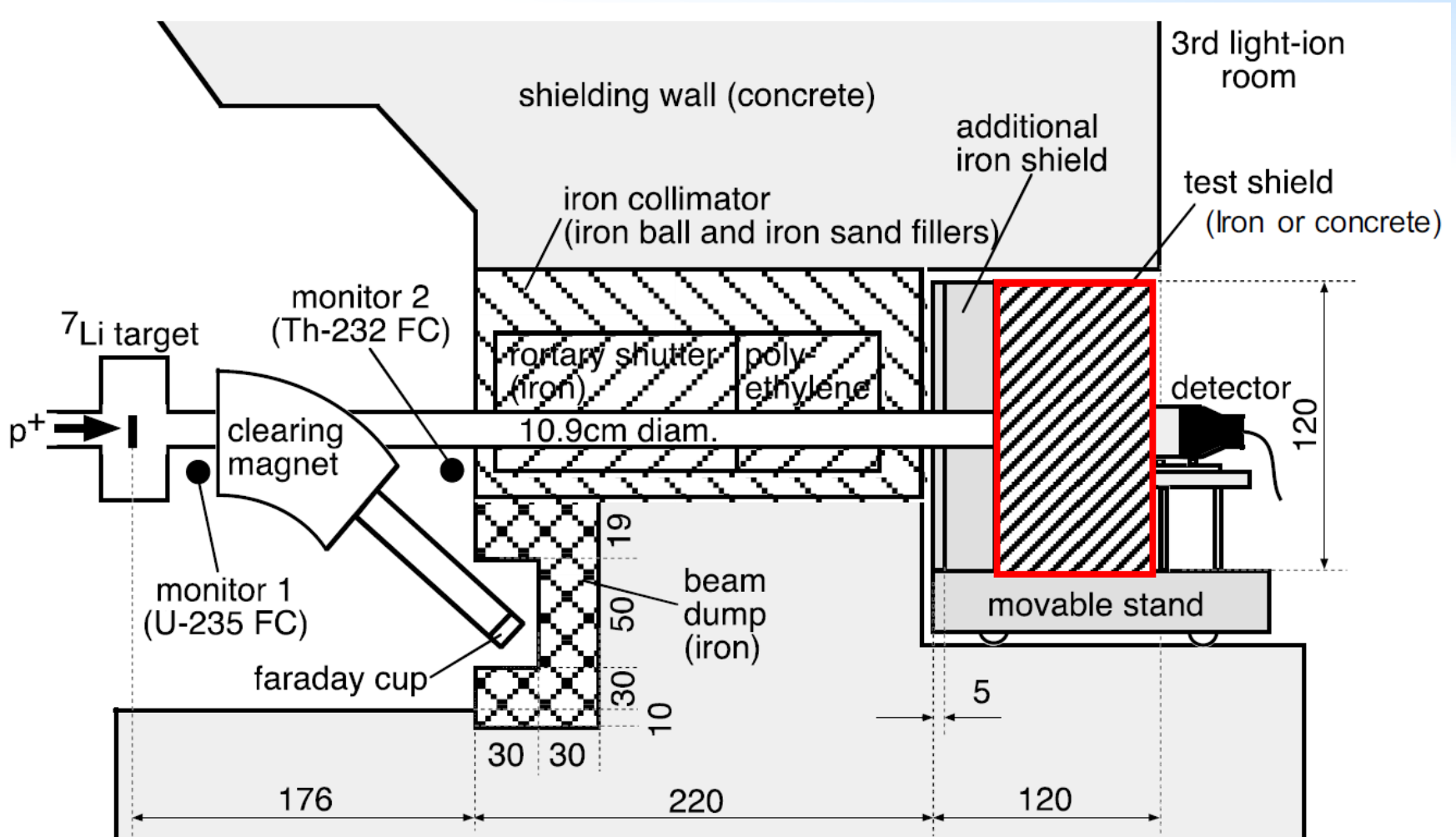
FNS-Fe Leakage Spectrum D-T Source
Fe_500_600_FNS_TOF 12.2 degrees



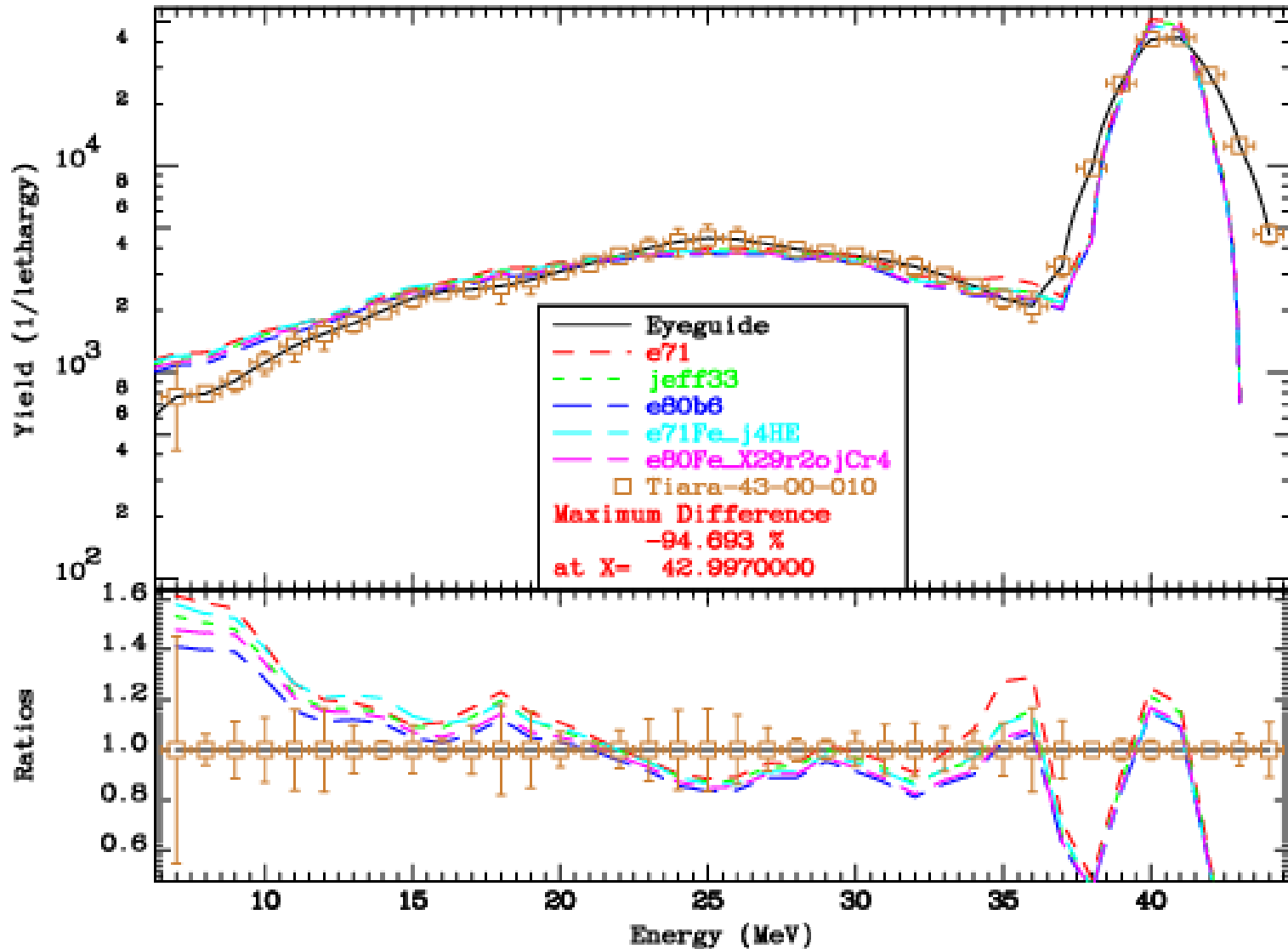
7. TIARA benchmark

- The 40 MeV and 65 MeV benchmarks are described in SINBAD, but no adequate MCNP models are available.
- Under contract with the IAEA, B. Kos (JSI, working with I. Kodeli) performed the analysis and delivered computational models for MCNP with weight-windows variance reduction
- The 40 MeV, 70 cm case has suspicious structure that is not observed with other spheres
- Agreement is less good for the 65 MeV case
- (Analysis of additional measured data is pending)

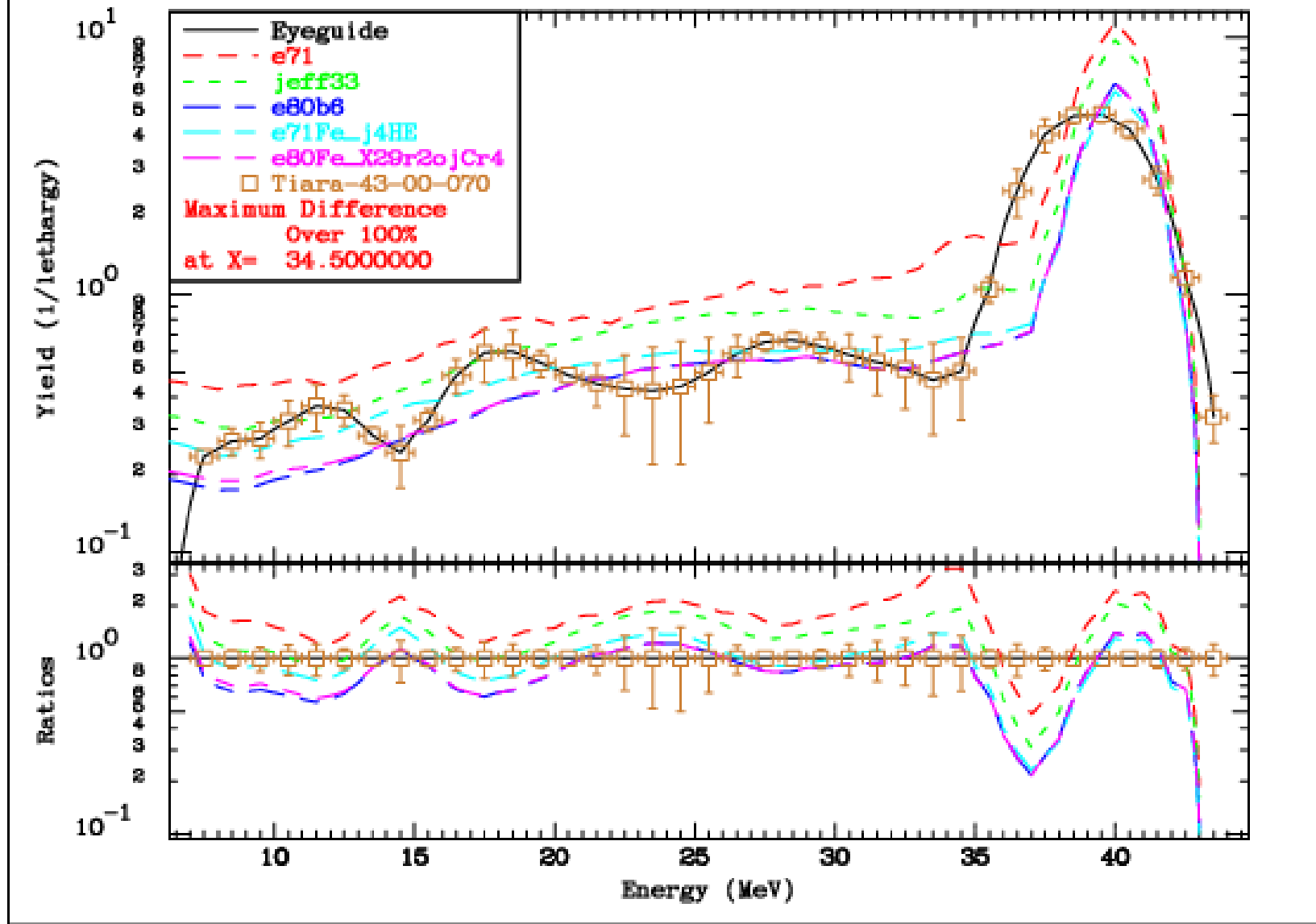
TIARA benchmark



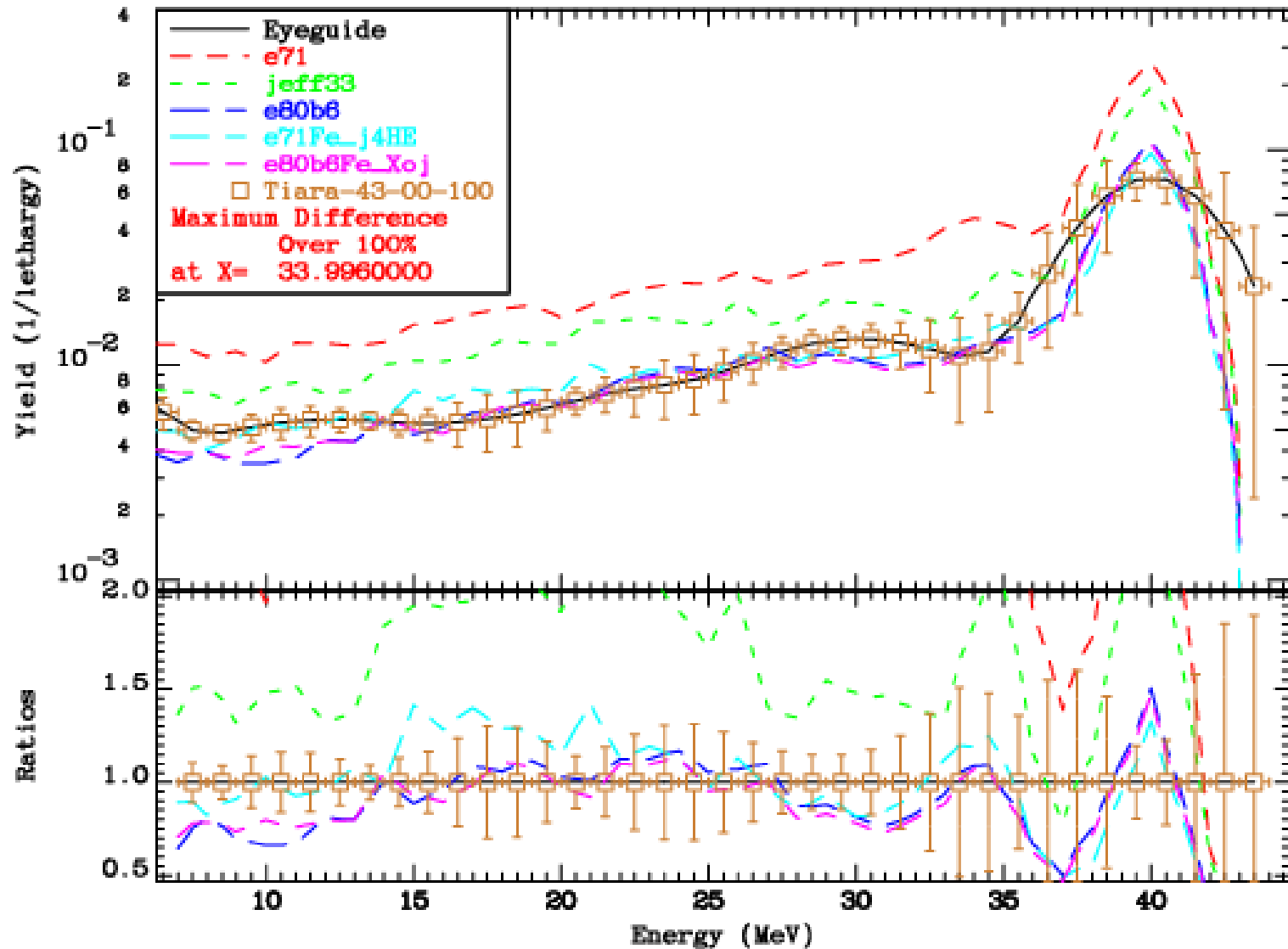
TIARA Leakage through Fe slab with p-Li Source
tiara-43-00-010



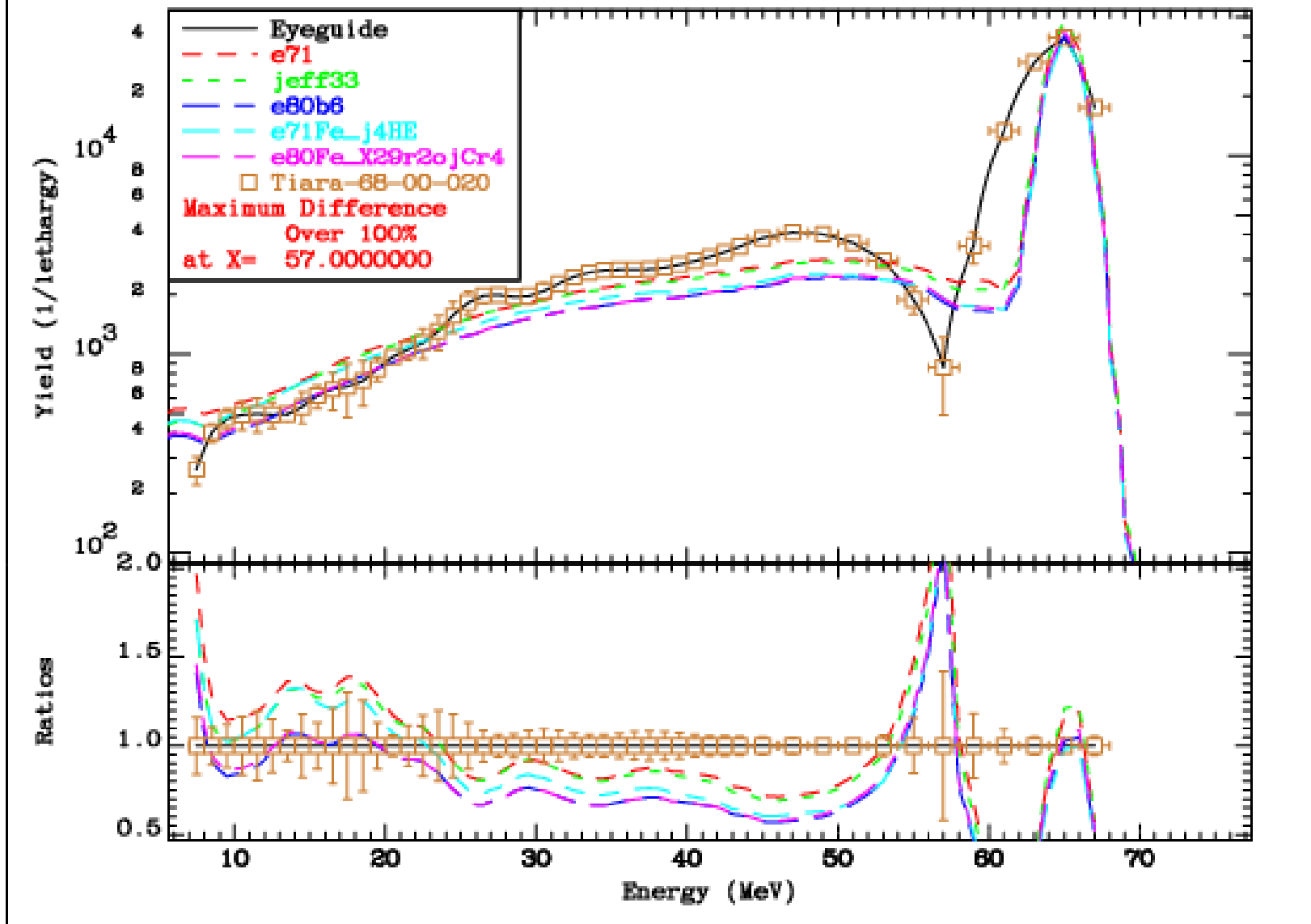
TIARA Leakage through Fe slab with p-Li Source
 tiara-43-00-070



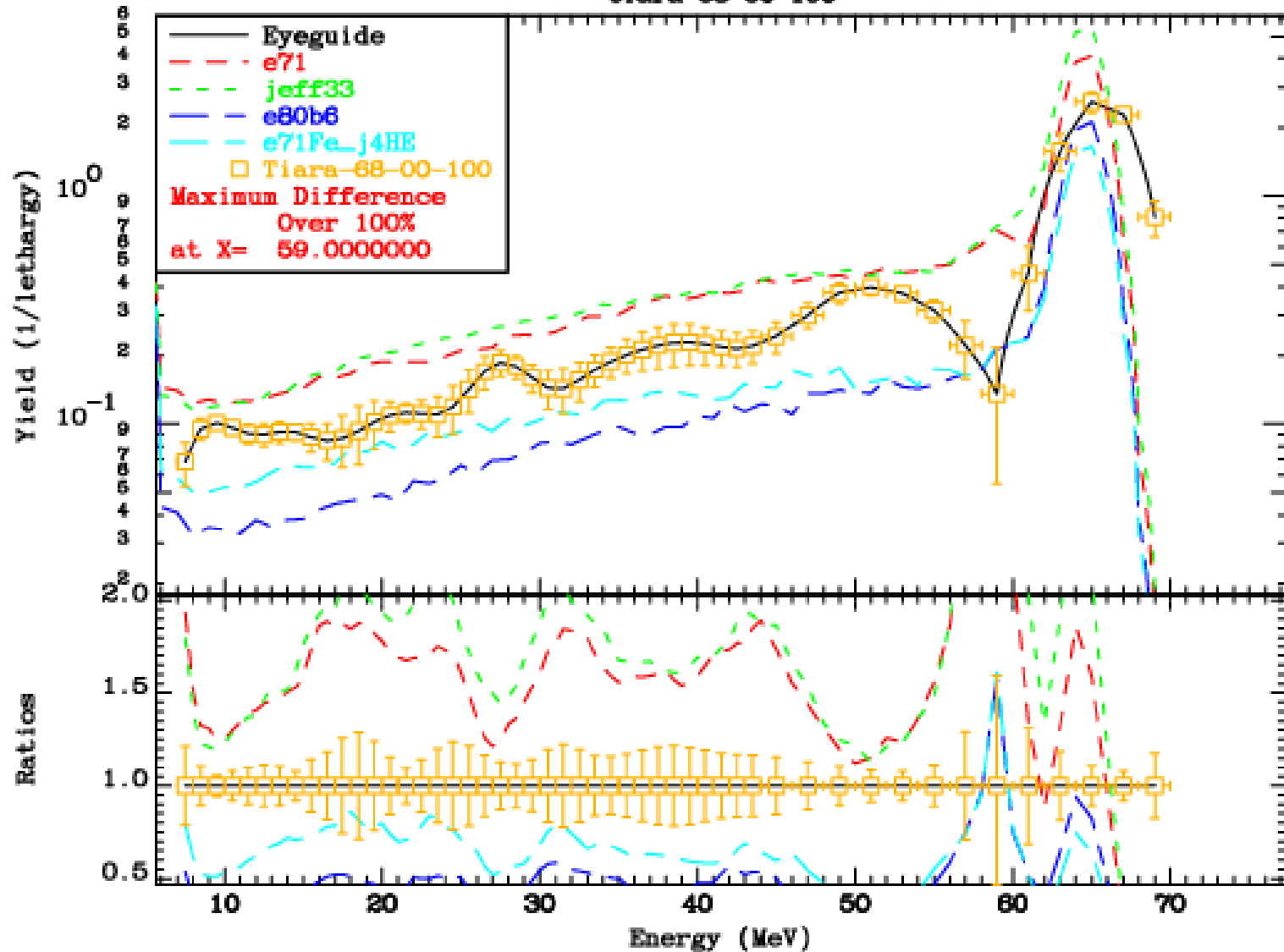
TIARA Leakage through Fe slab with p-Li Source
tiara-43-00-100



TIARA Leakage through Fe slab with p-Li Source
tiara-68-00-020



TIARA Leakage through Fe slab with p-Li Source
tiara-68-00-100



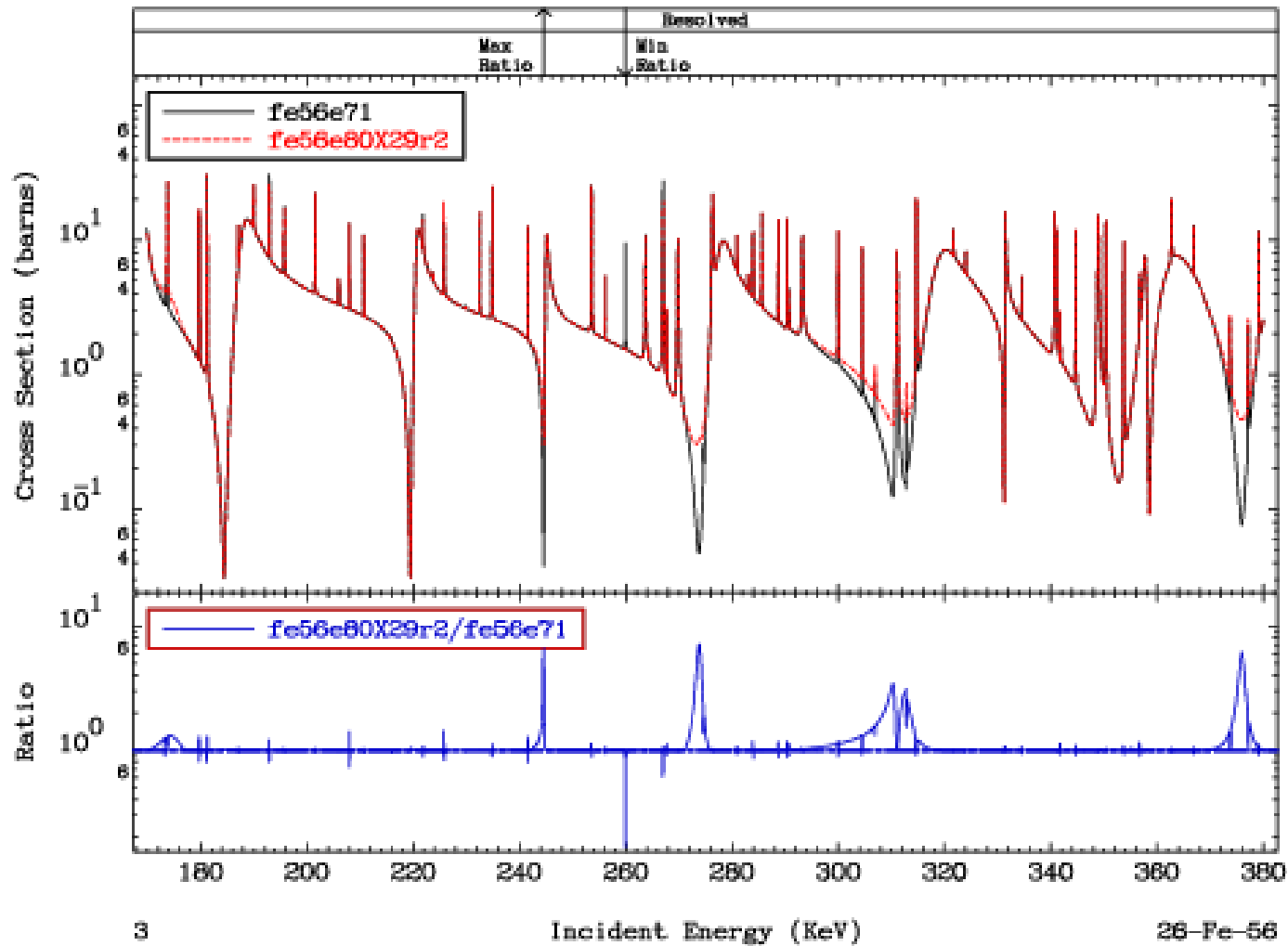
8. IPPE Fe broomstick experiments with p-T source

- Transmission of quasi-monoenergetic neutrons from a p-T source through iron cylinders of different thicknesses
- “Detailed” results pointed to elastic x.s. deficiencies in the resonance minima at:
 - 174 keV 1.0 b (0 at 170, 177 keV)
 - 244 keV 0.3 b (0 at 242, 245 keV)
 - 267 keV -10 b (0 at 266.95, 267.1 keV)
 - 274 keV 0.3 b (0 at 271, 276 keV)
 - 310-313 keV 0.3 b (0 at 290, 320 keV)
 - 376 keV 0.3 b (0 at 370, 380 keV)
 - 1.02 MeV 0.1 b (from 0 at 0.85 MeV)
 - 1.40 MeV -0.15 b
 - 1.60 MeV 0.10 b
 - 1.90 MeV -0.20 b (to 0 at 2.0 MeV)

MAT 2631

Elastic
Cross Section

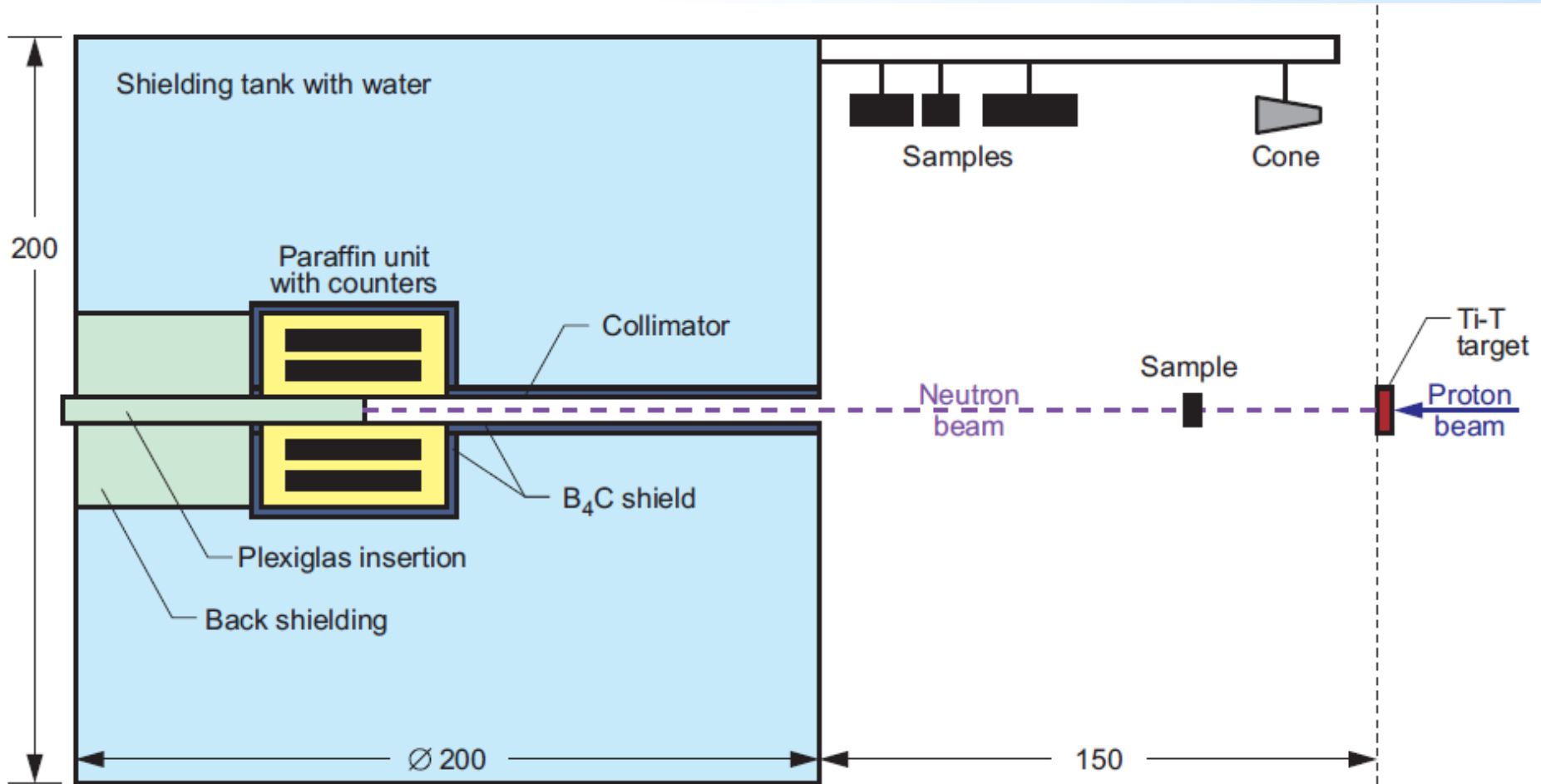
²⁶Fe-56
-83.54 To 742.6 %



3

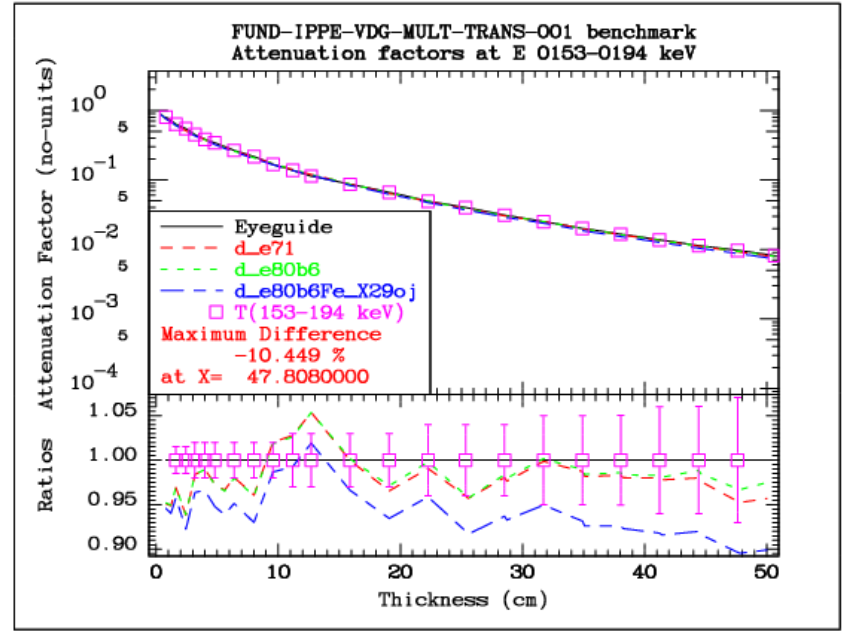
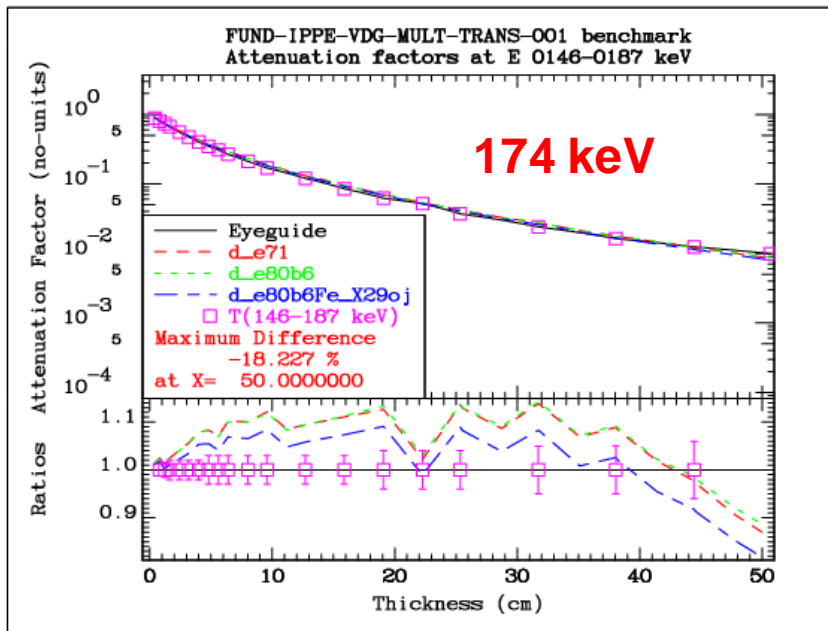
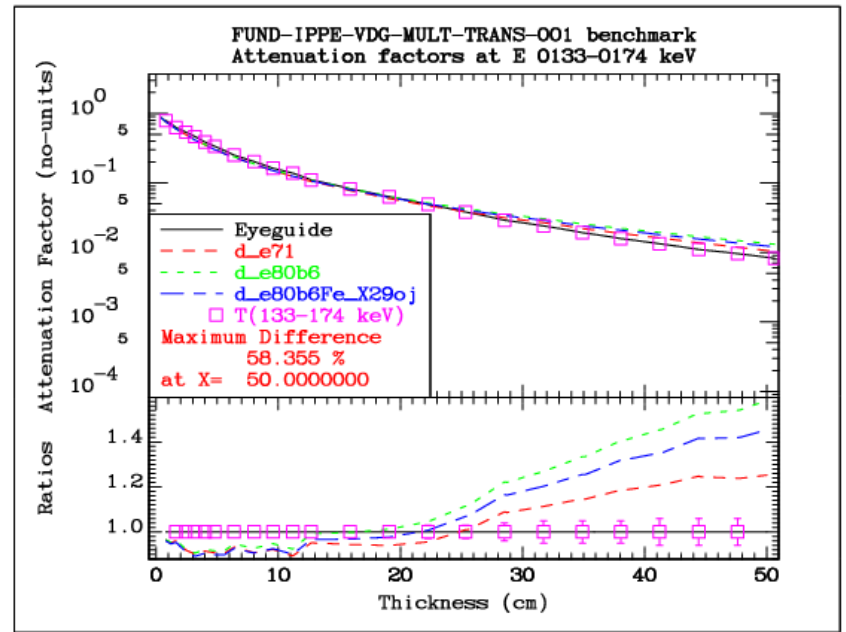
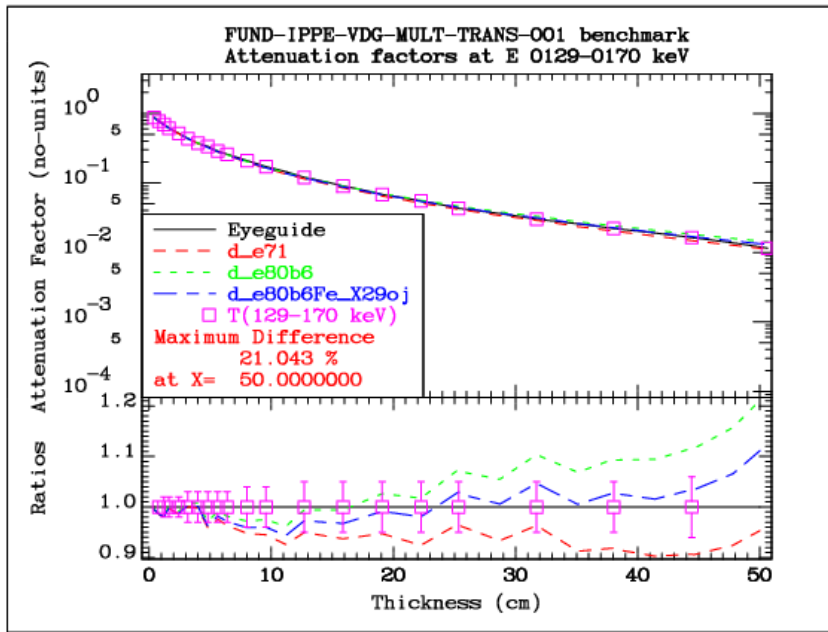
²⁶Fe-56

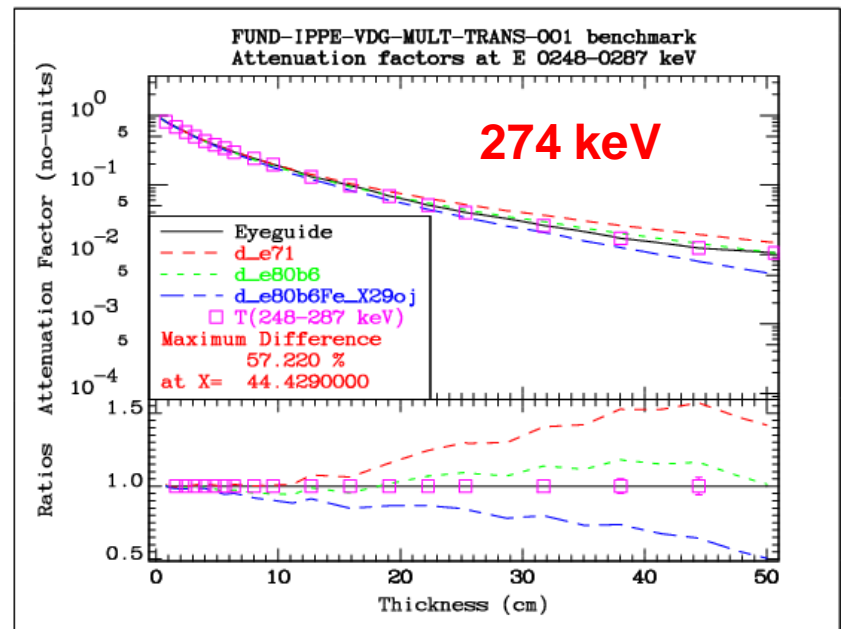
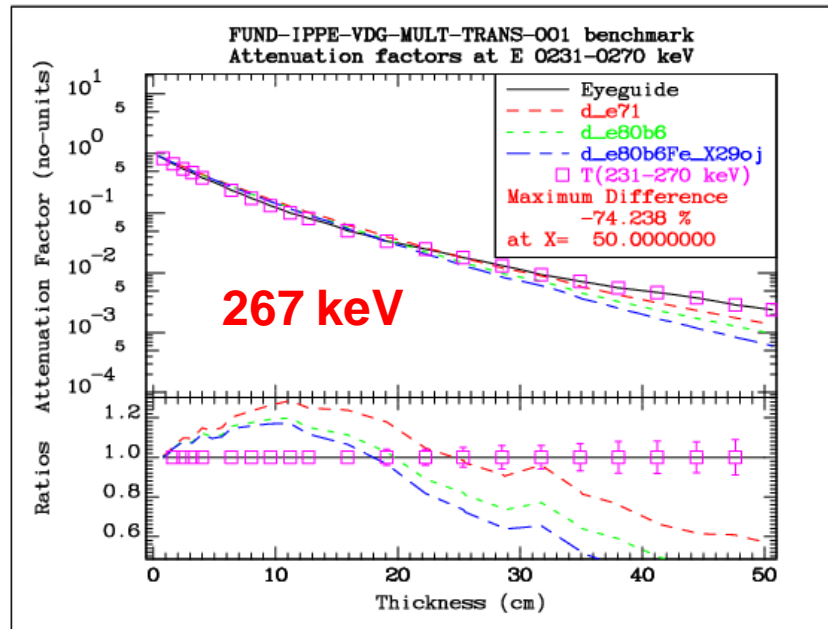
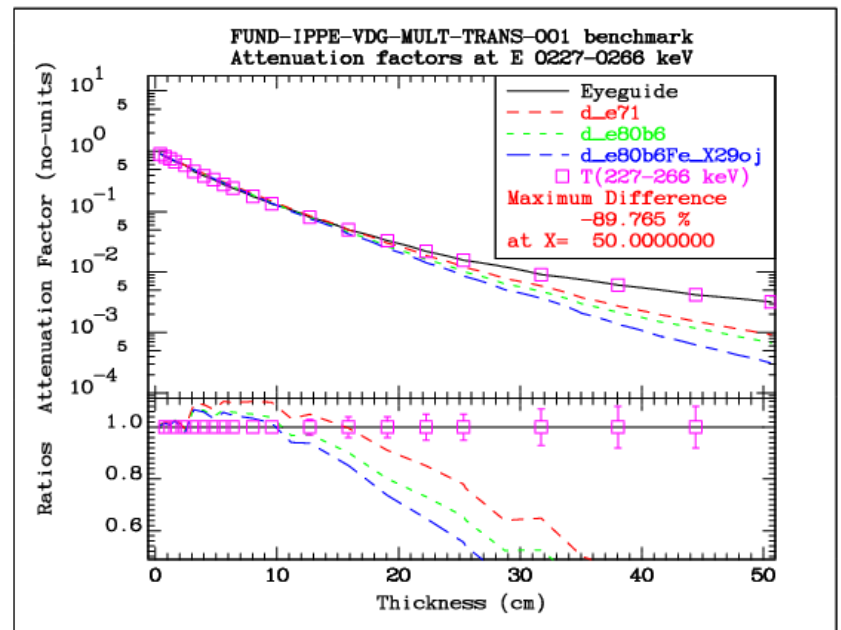
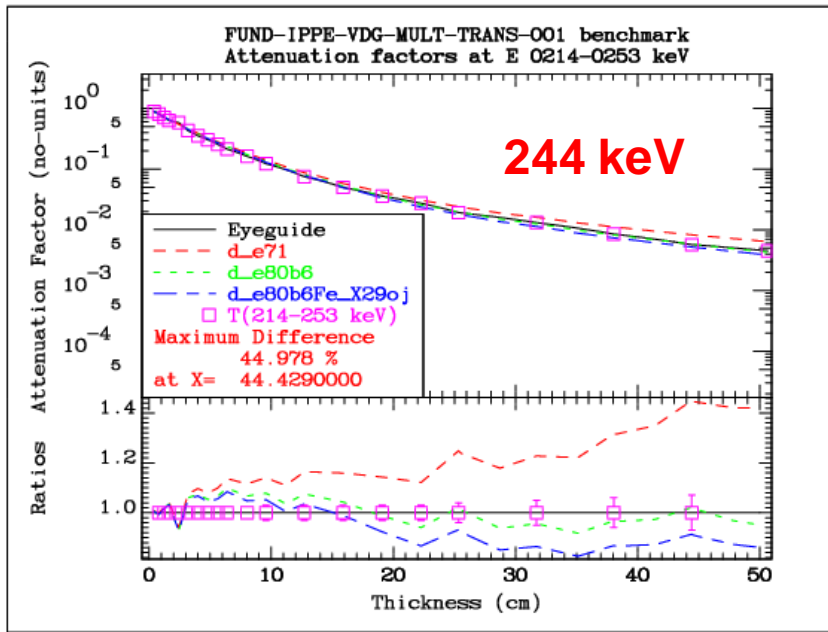
IPPE Fe broomstick experiments with p-T source

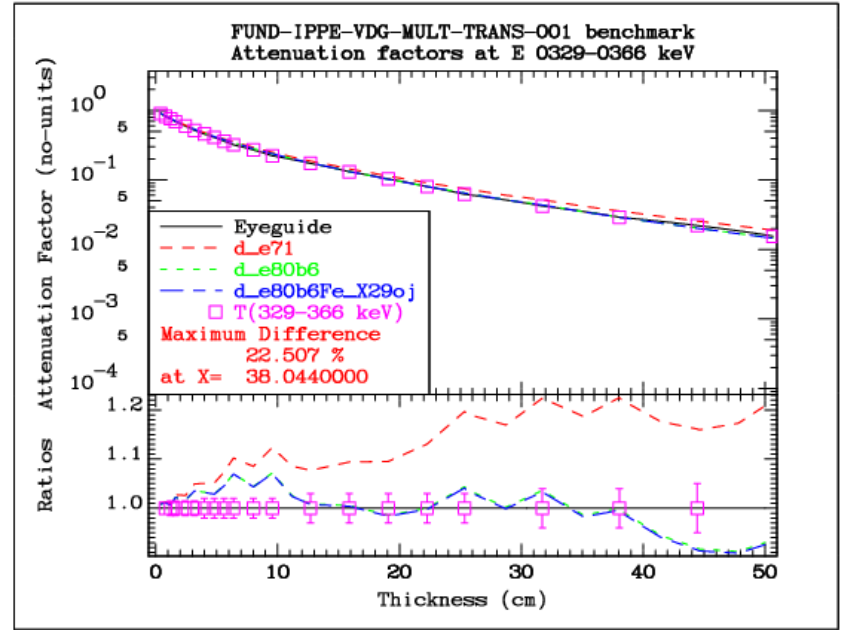
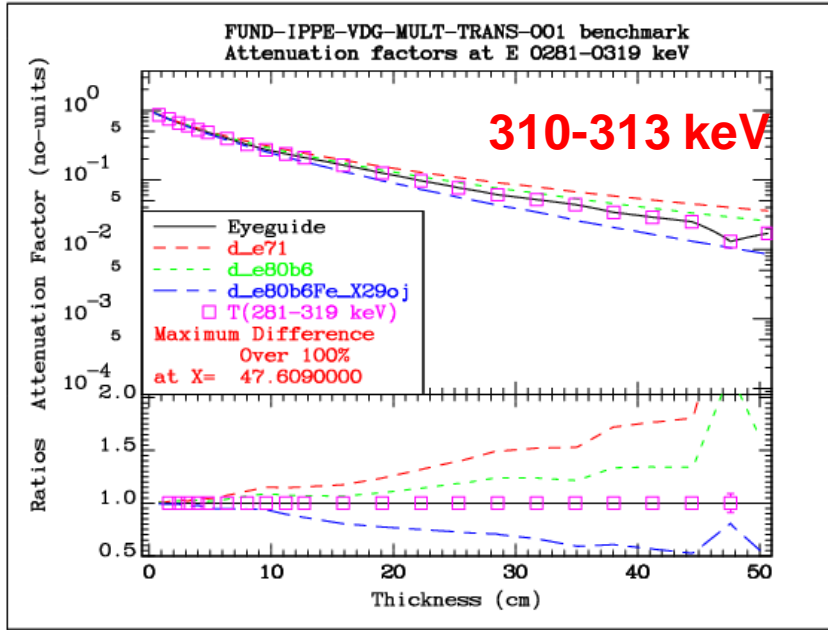
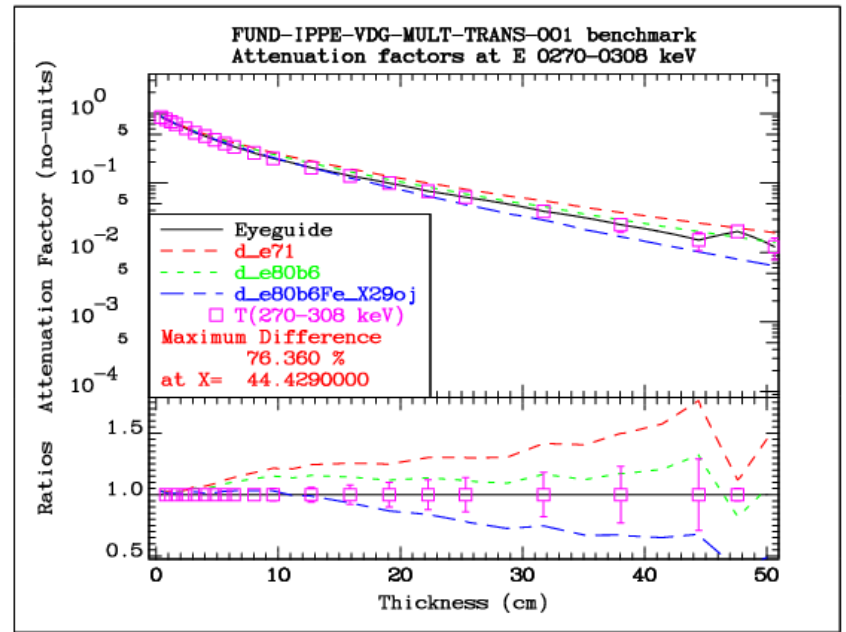
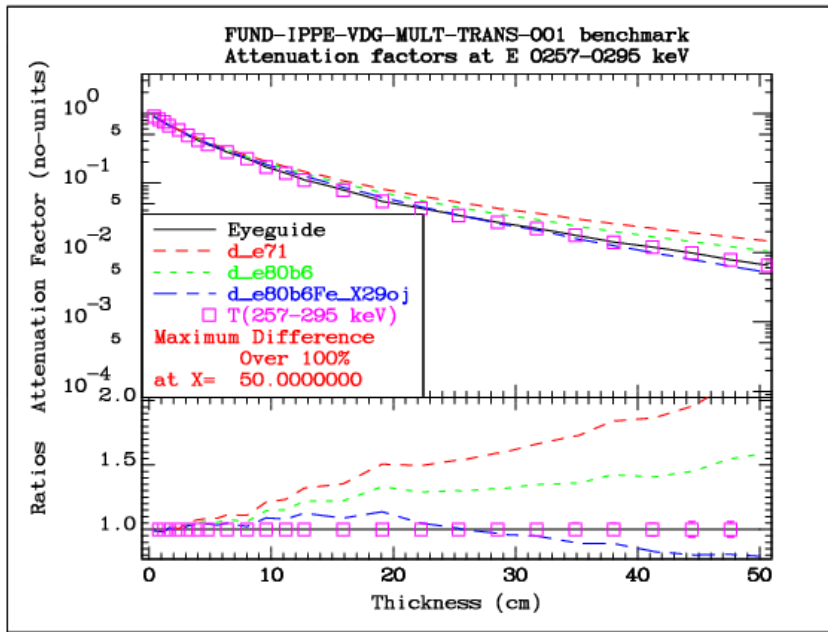


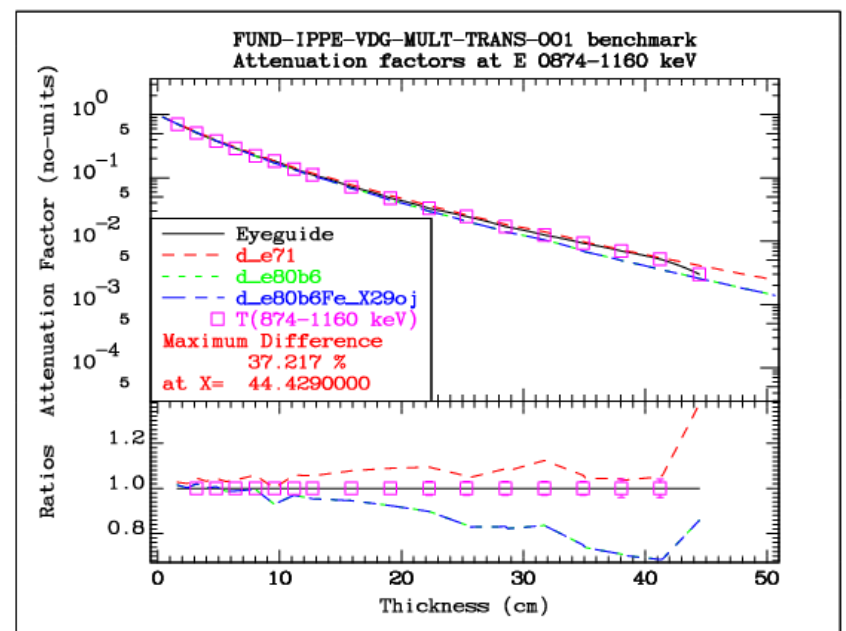
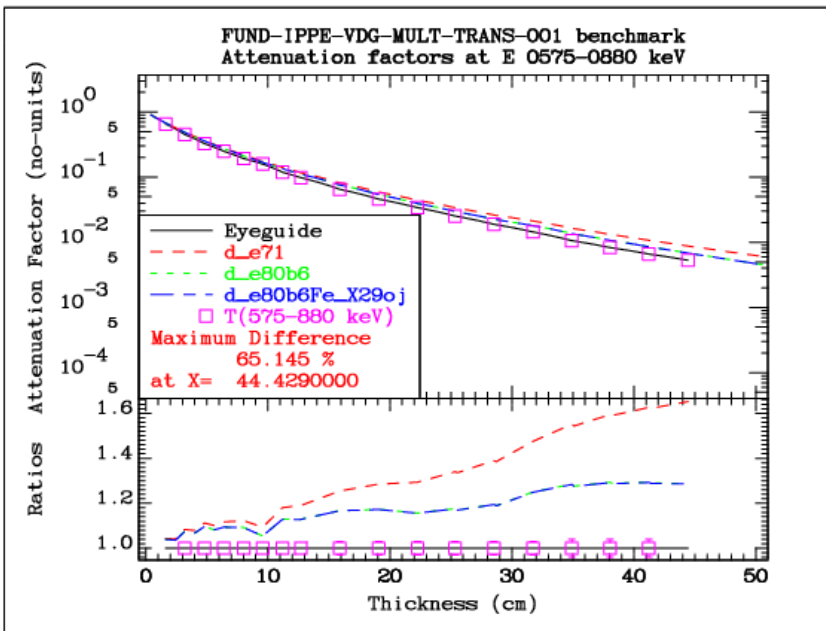
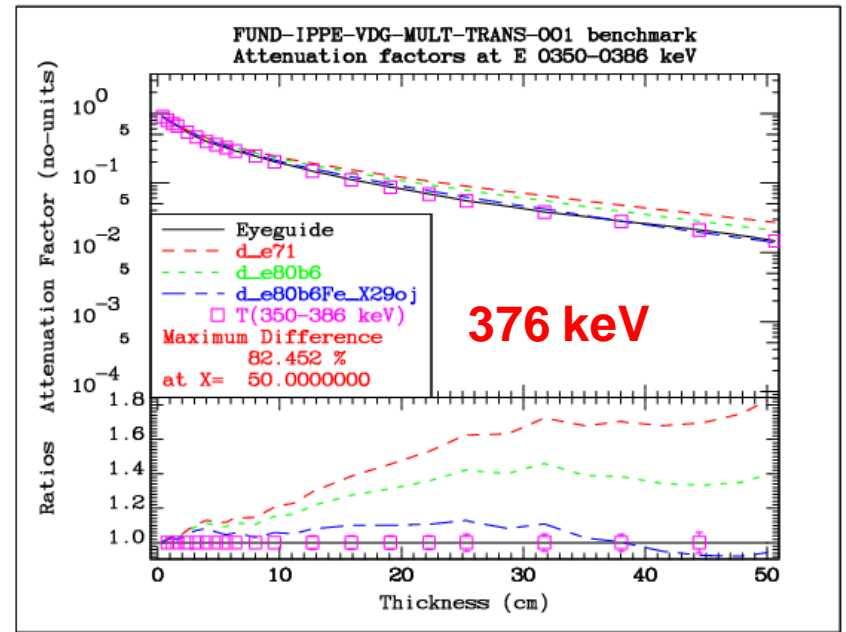
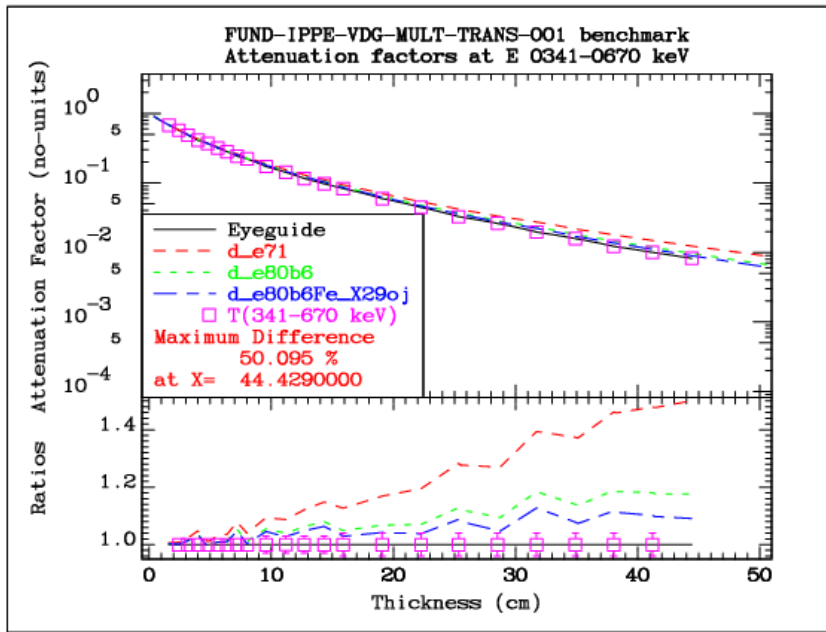
Dimensions in cm

08-GA50017-174-1





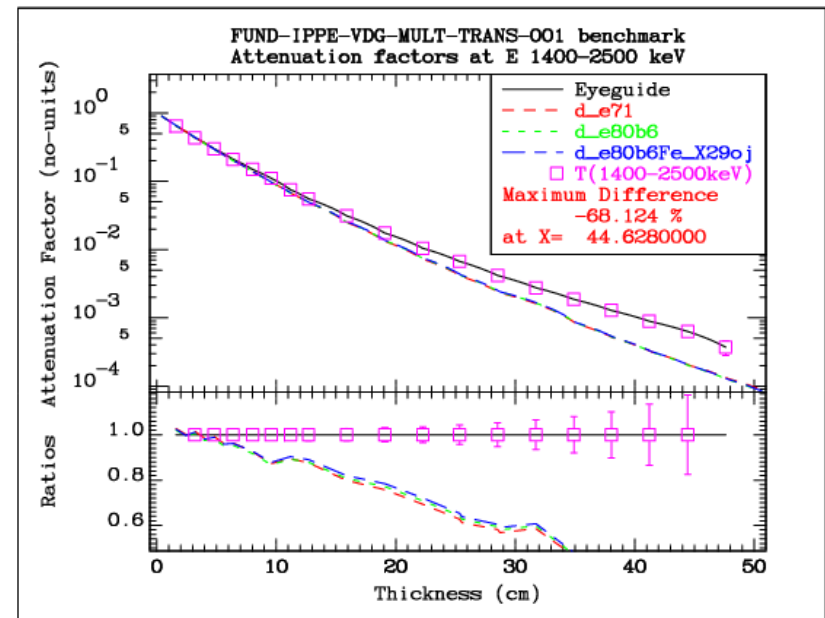
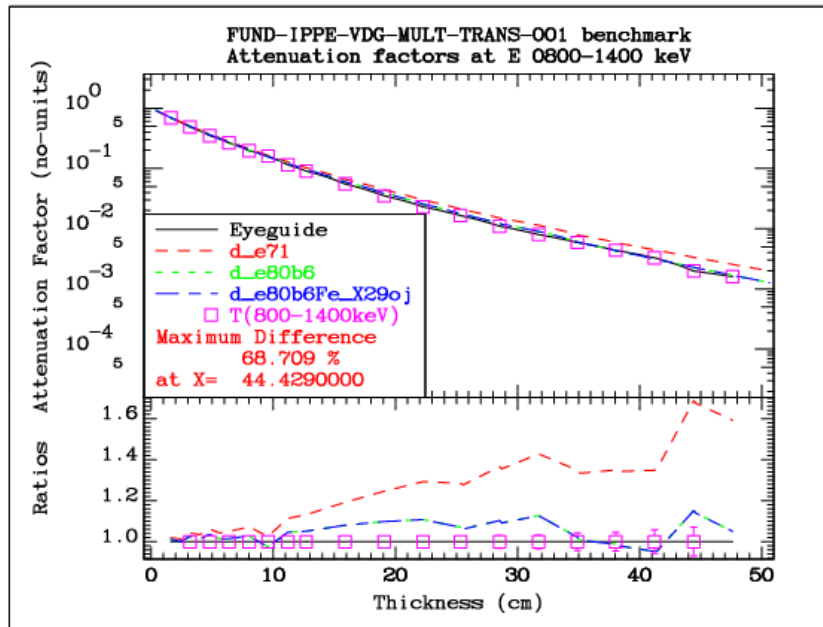
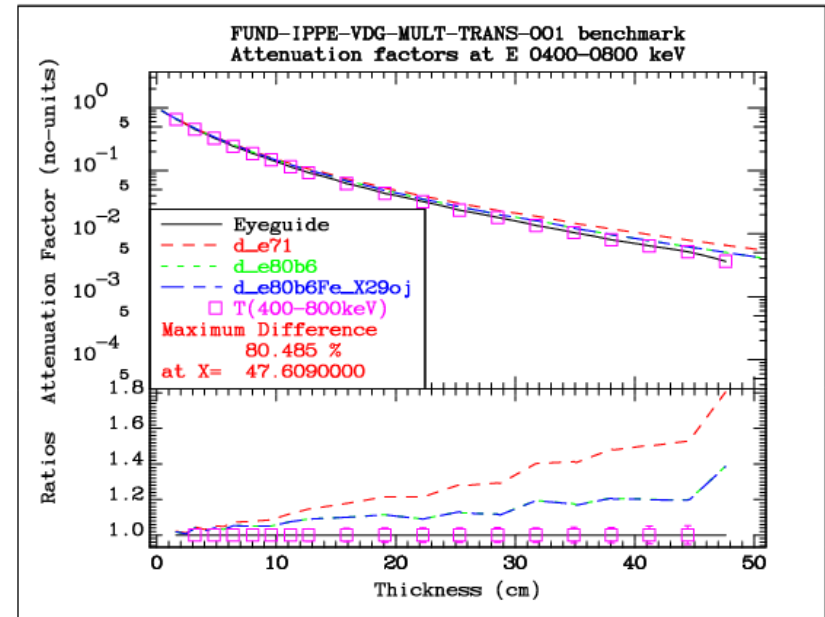
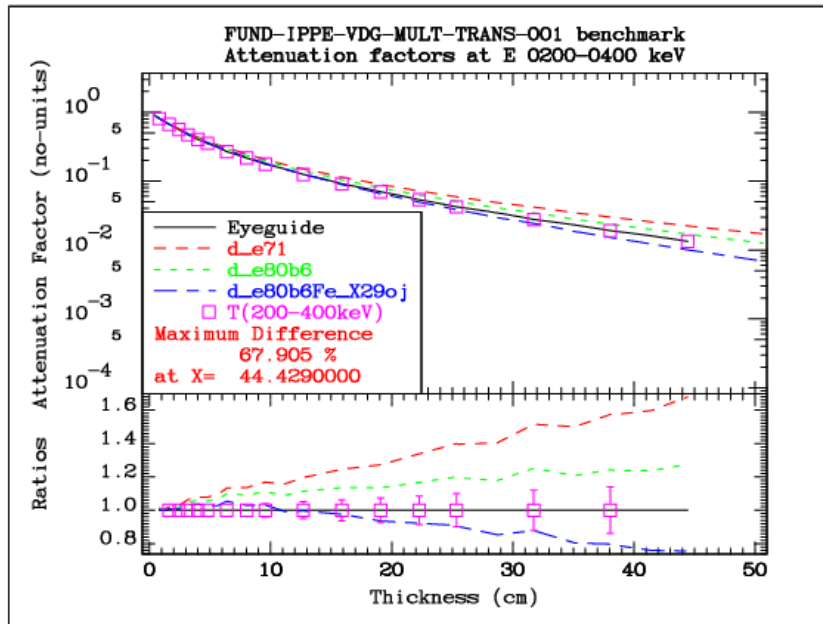




IPPE Fe broomstick experiments with p-T source (cont.)

Coarse energy grid:

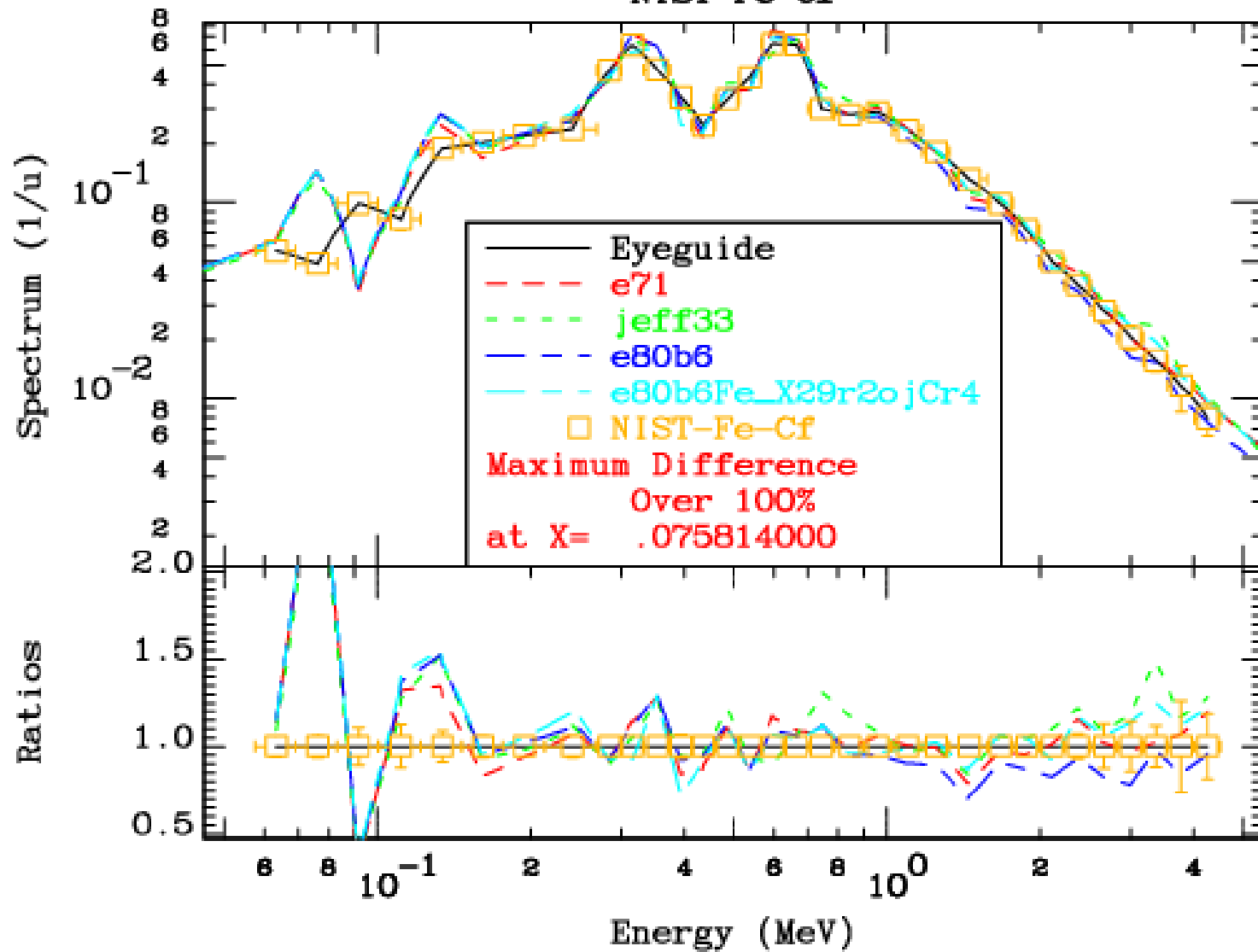
- Based on this benchmark better agreement with measured data was achieved with the new data in cases, where the dips in the elastic were responsible for the mismatch at energies below ~ 1.2 MeV
- At higher energies the calculated attenuation is larger with all libraries
- Due to high anisotropy at these energies the attenuation is governed by the non-elastic cross section
- The required decrease in the non-elastic cross section can not be supported by differential data. Possible effects:
 - Downscattering?
 - Room return?
 - Source modelling?



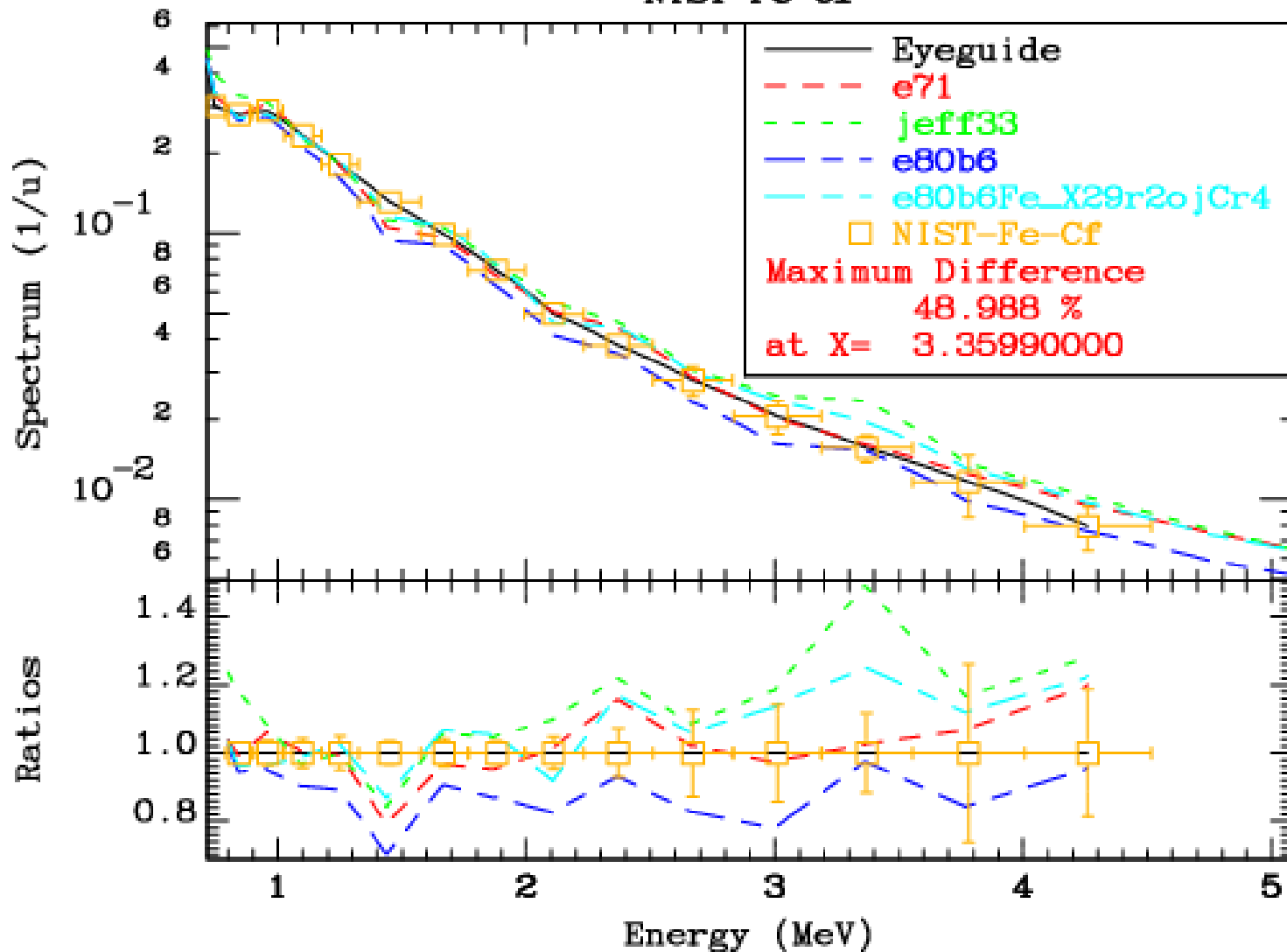
NIST Fe sphere with Cf source

- The benchmark is similar to the IPPE benchmark
- The measured data are consistent with IPPE but too coarse to add to the information

NIST-Fe Sphere Leakage Spectrum NIST-Fe-Cf



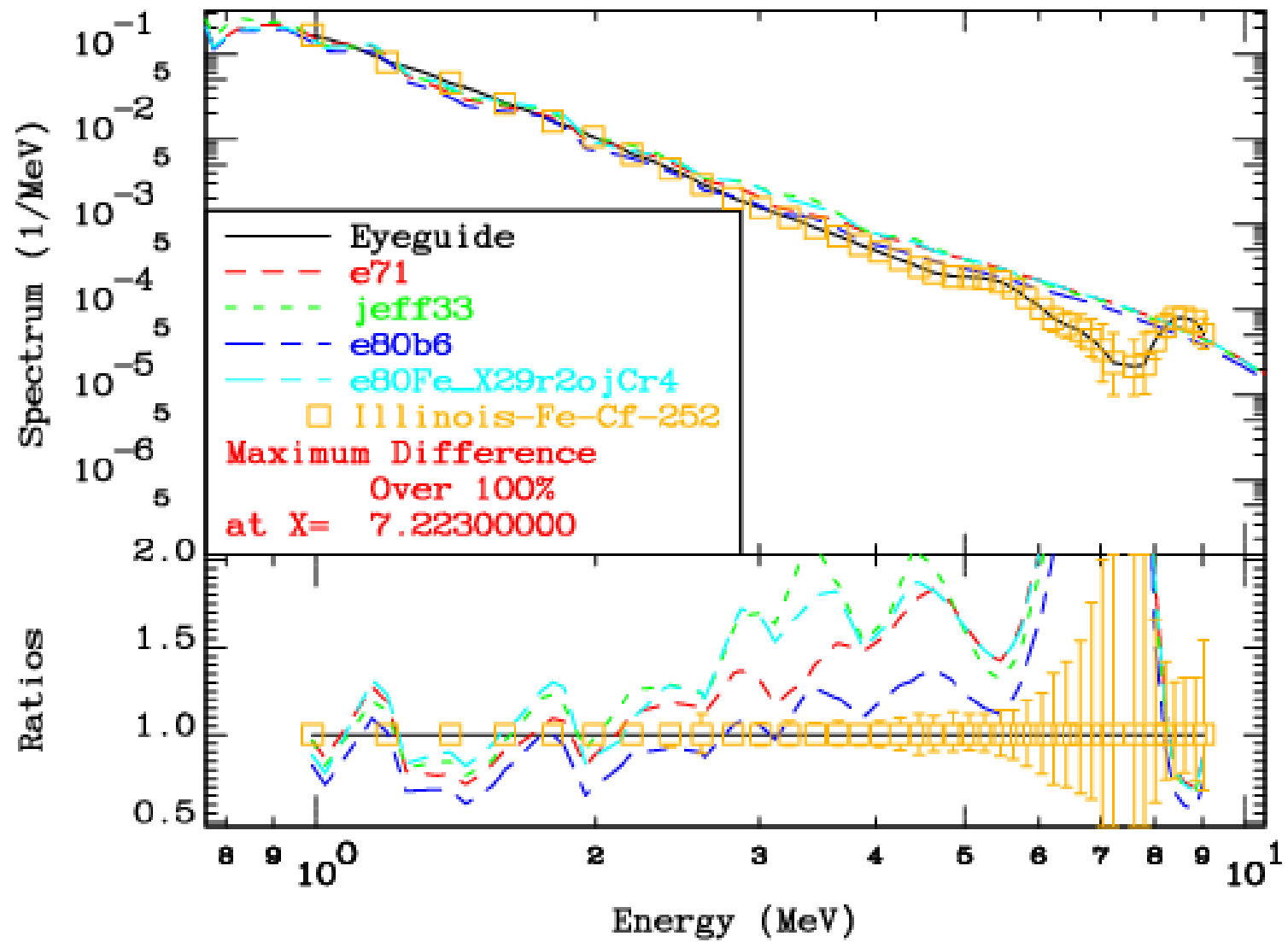
NIST-Fe Sphere Leakage Spectrum NIST-Fe-Cf



Illinois Fe sphere with Cf source

- The benchmark is similar to the IPPE benchmark; Fe sphere diameter is 38.1 cm
- The structure in the measured spectrum above 6 MeV seems unphysical
- At lower energies the measured data are consistent with IPPE but too coarse to add to the information

Illinois-Fe Sphere Leakage Spectrum ILLN-Fe-Cf



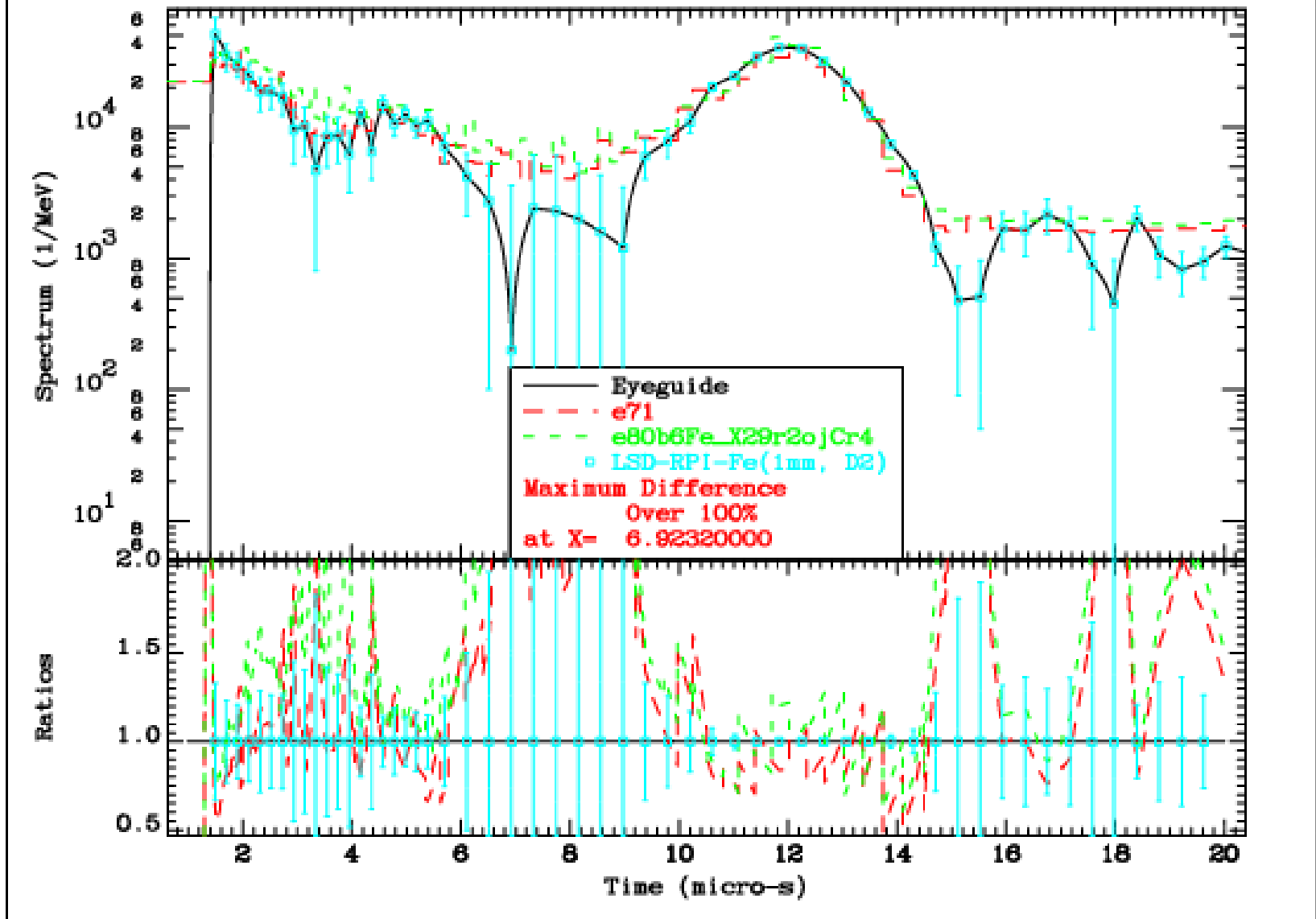
EURACOS deep penetration benchmark

- The benchmark is similar to the ASPIS-Fe88 benchmark
- The source configuration is not well defined, making the results less reliable
- (Calculations were not repeated with the latest data file)

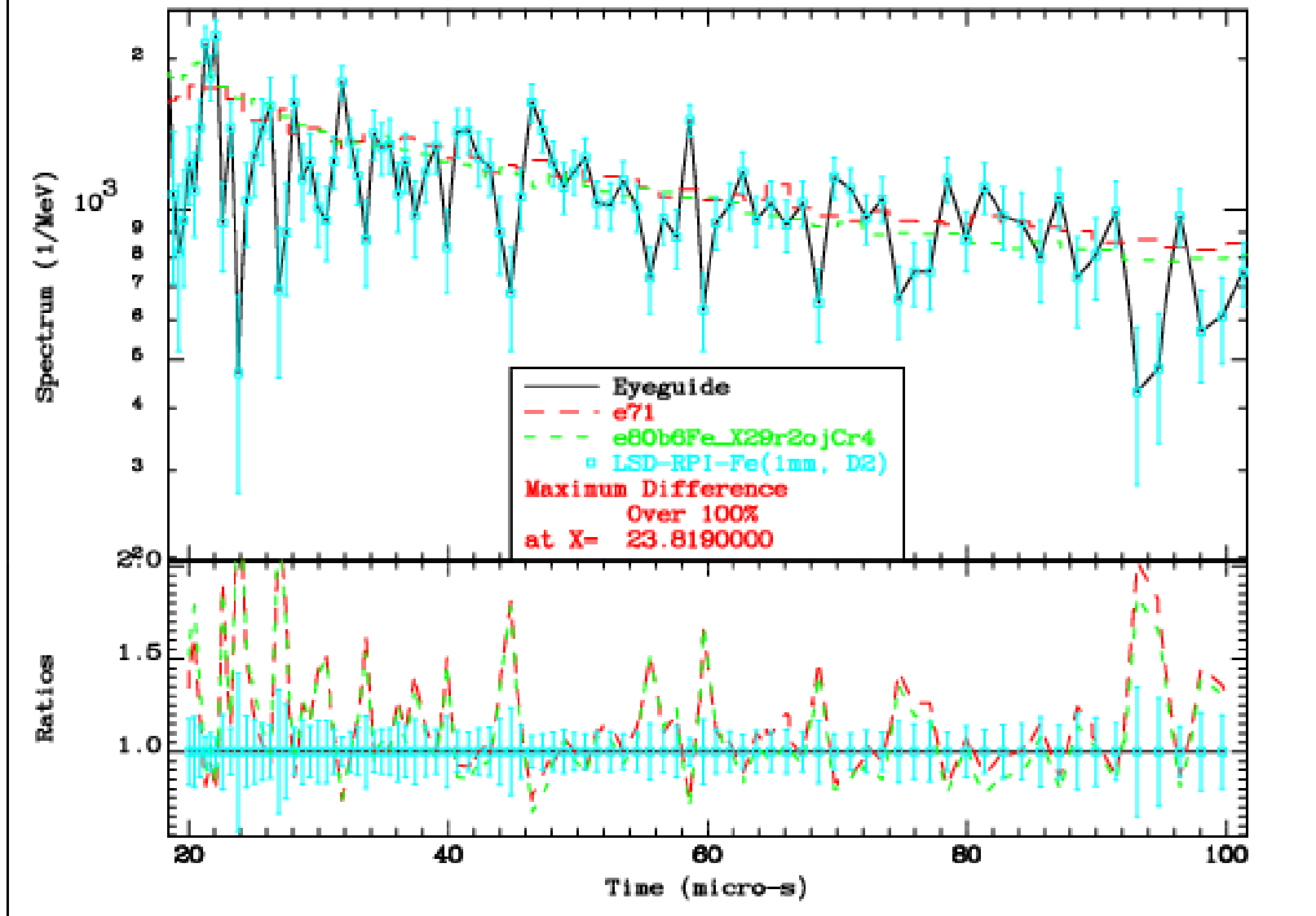
RPI lead-slowing-down benchmark

- The benchmark could be valuable for low-resolution cross section validation
- Unfortunately, the statistical scattering of measured data is too large to be of any use

LSD-RPI Lead Slowing-Down Benchmark
LSD-RPI-Fe



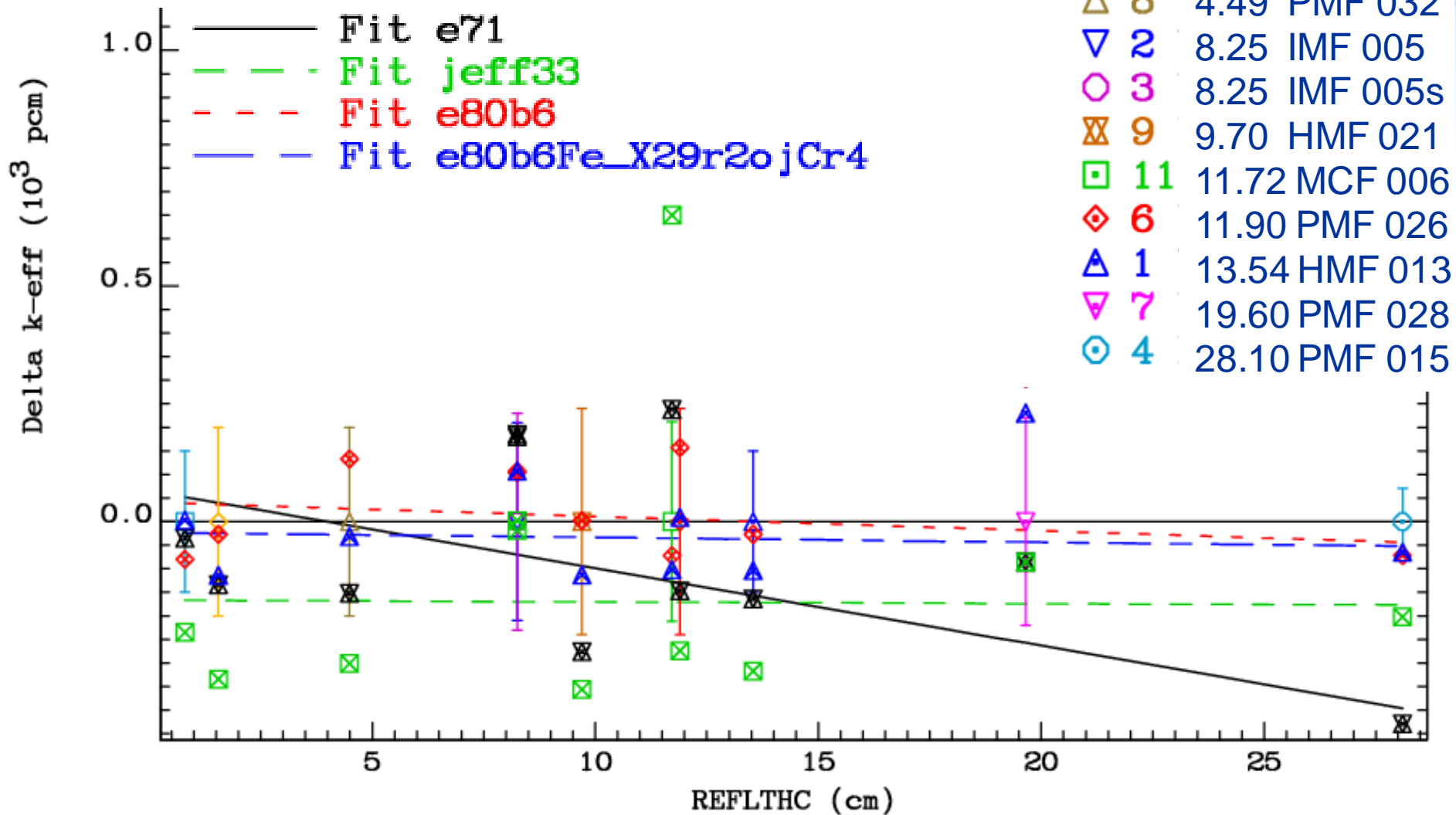
LSD-RPI Lead Slowing-Down Benchmark
LSD-RPI-Fe



Criticality benchmarks

- Good performance in criticality benchmarks was retained
- Lower thermal capture in ^{56}Fe improves Russian FKBN-2 benchmarks (hmf088), but makes IPEN/MB-01 slightly worse
- Planet-Fe/PE benchmarks are Fe/PE like FKBN-2, but most Planet benchmarks with PE are systematically predicted high
- The ZPR-4/59 (pmi004) is lead-reflected; there seem to be problems with many benchmarks involving Pb
- The big improvement in ZPR-6/10 is mainly due to a trial change to the ^{53}Cr capture data in the triplet of strong resonances near 5 keV

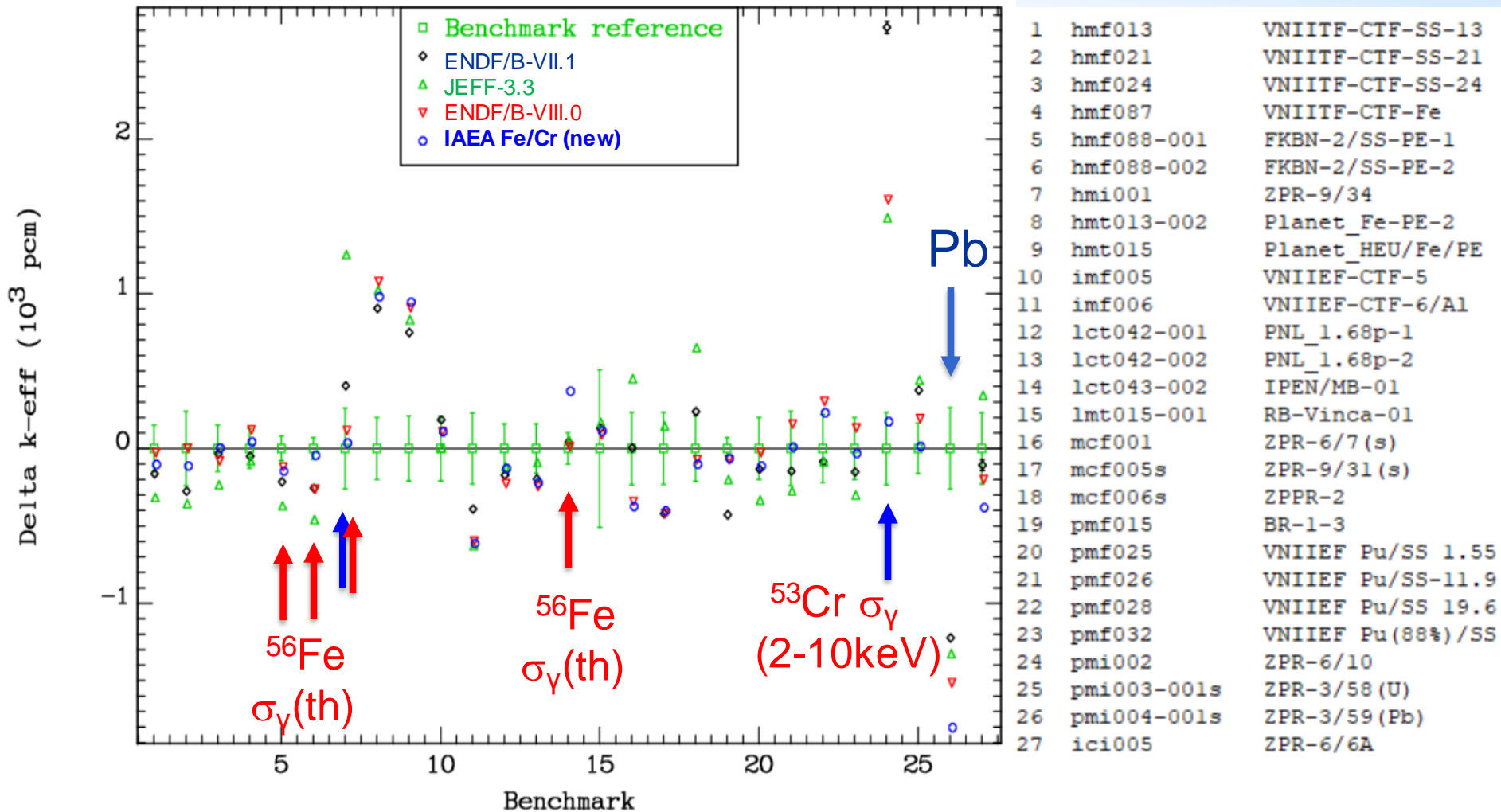
Iron benchmarks (refl)



Criticality impact of $^{56}\text{Fe}/^{53}\text{Cr}$



ICSBEP Benchmarks Sensitive to Iron
Integral Parameter Intercomparison



Conclusions regarding ^{56}Fe

- Problems identified in the CIELO evaluation were largely removed, while retaining good performance in criticality calculations.
- IAEA INDEN ^{56}Fe evaluation is a significant improvement over CIELO and ENDF/B-VII.1 evaluations.
- The new evaluation is available and could be a candidate for updating current libraries.
- However, this is patching. Consistent solution of the problems is needed.



IAEA

International Atomic Energy Agency

Atoms for Peace and Development

Thank you!

