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Identifying gaps in Critical Benchmarks through Analysis of Sensitivities

Nicholas Thompson

Institut de Radioprotection et de Sûreté Nucléaire (IRSN)

Los Alamos National Laboratory (LANL)

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Let's start from the beginning

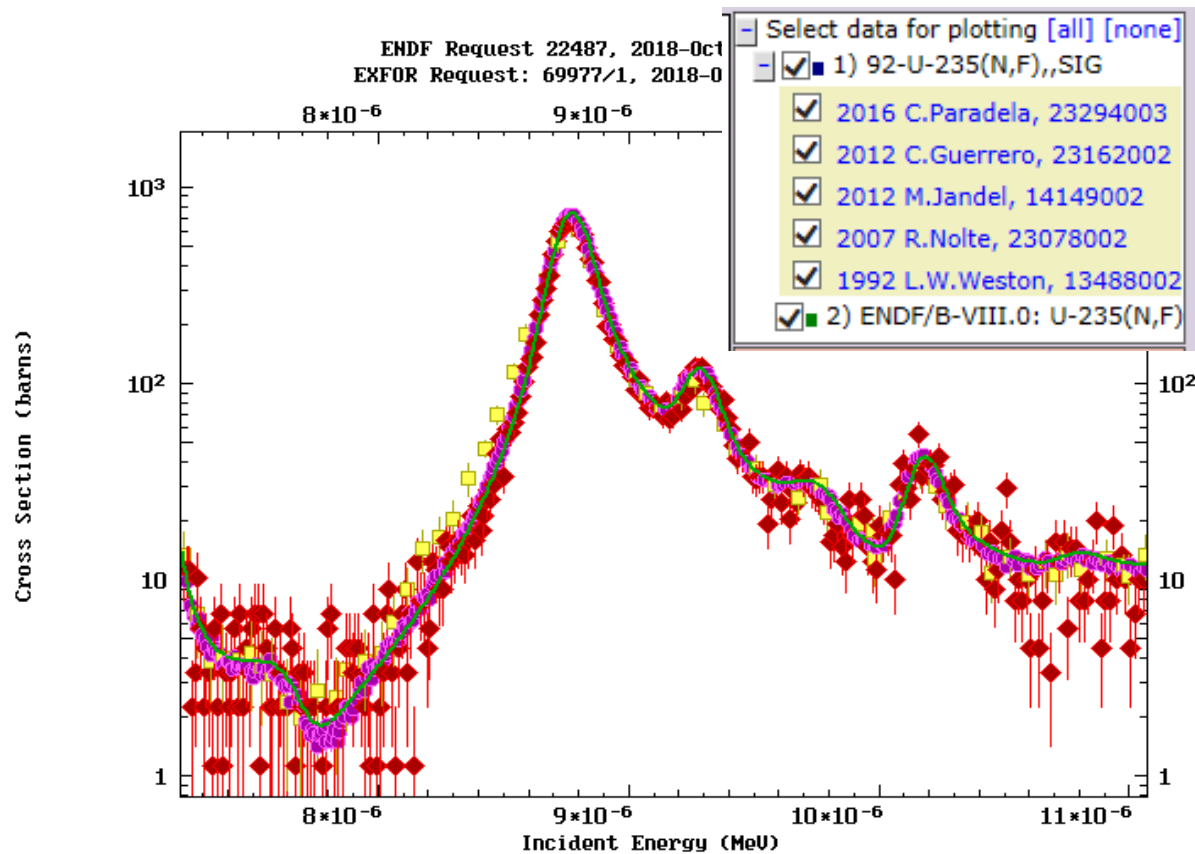
- **Who uses nuclear data?**
- **Have you ever run a simulation, and it doesn't match experiments/doesn't match what you expect?**
 - What did you do?
 - Check geometry, check materials, densities, options, etc.
 - Is nuclear data the problem? **What do you do then?**
 - Ask someone who knows nuclear data?
 - Try to dig into the data yourself?
- **How is nuclear data made?**

“Life cycle” of nuclear data

- Measurements are made

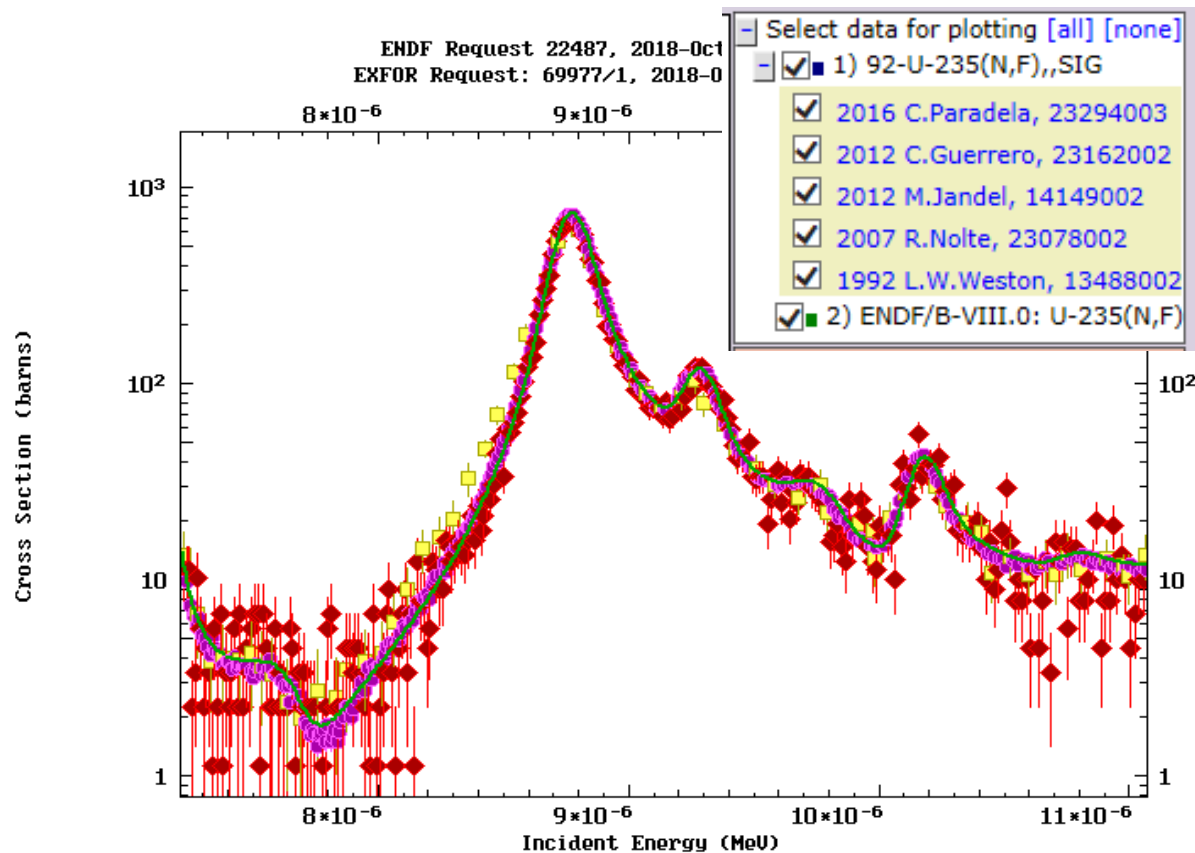
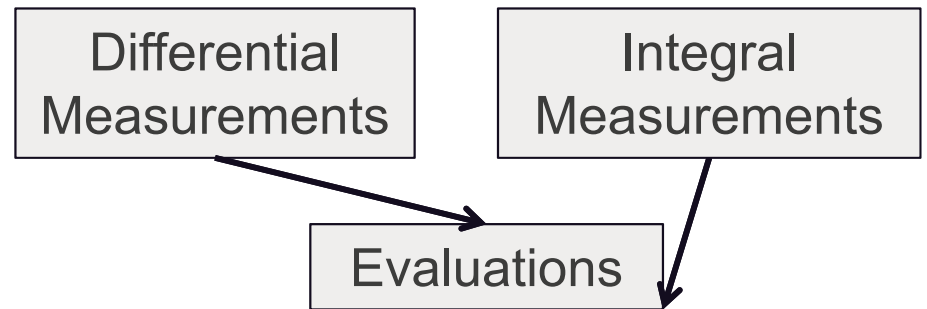
Differential
Measurements

Integral
Measurements



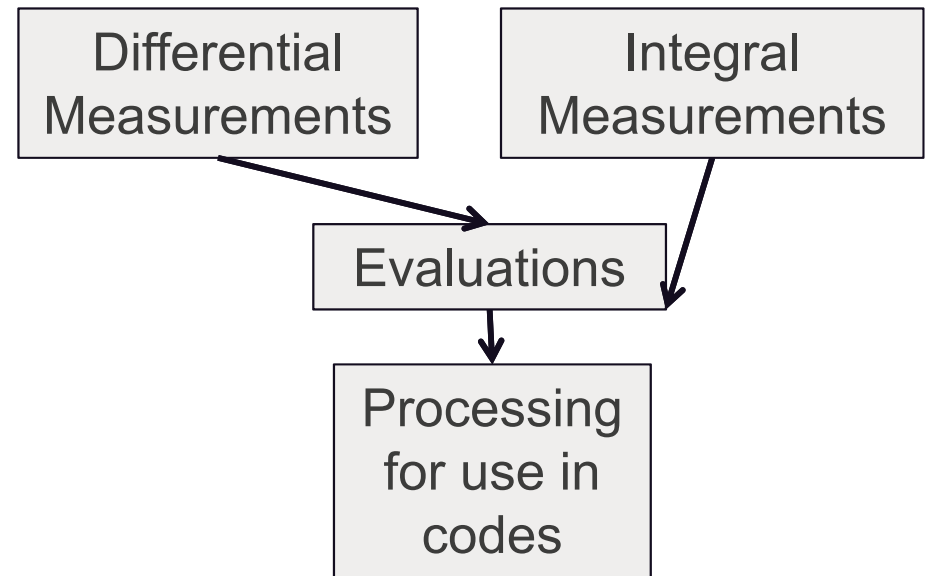
“Life cycle” of nuclear data

- Measurements are made
- Evaluators use those measurements



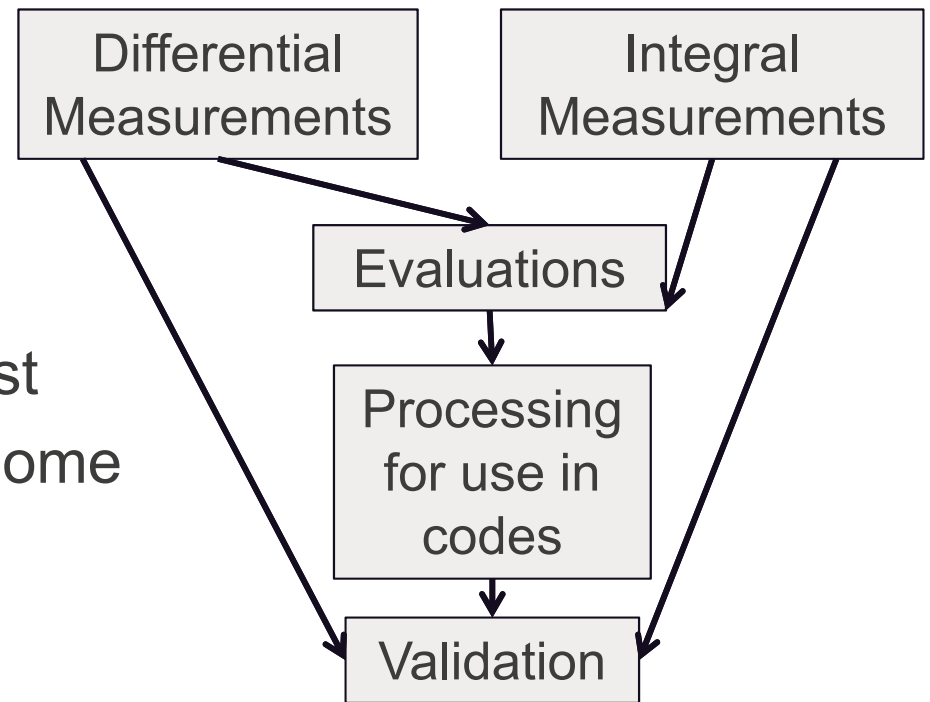
“Life cycle” of nuclear data

- Measurements are made
- Evaluators use those measurements
- Evaluations are processed



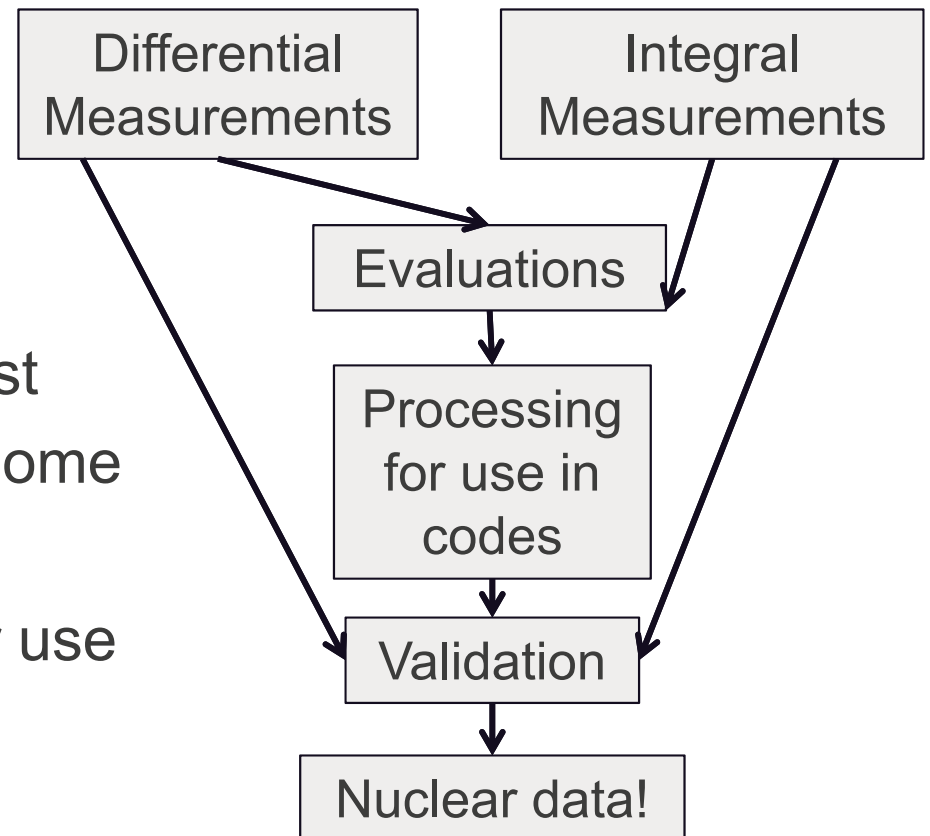
“Life cycle” of nuclear data

- Measurements are made
- Evaluators use those measurements
- Evaluations are processed
- Processed data is validated against integral measurements (and some differential measurements)



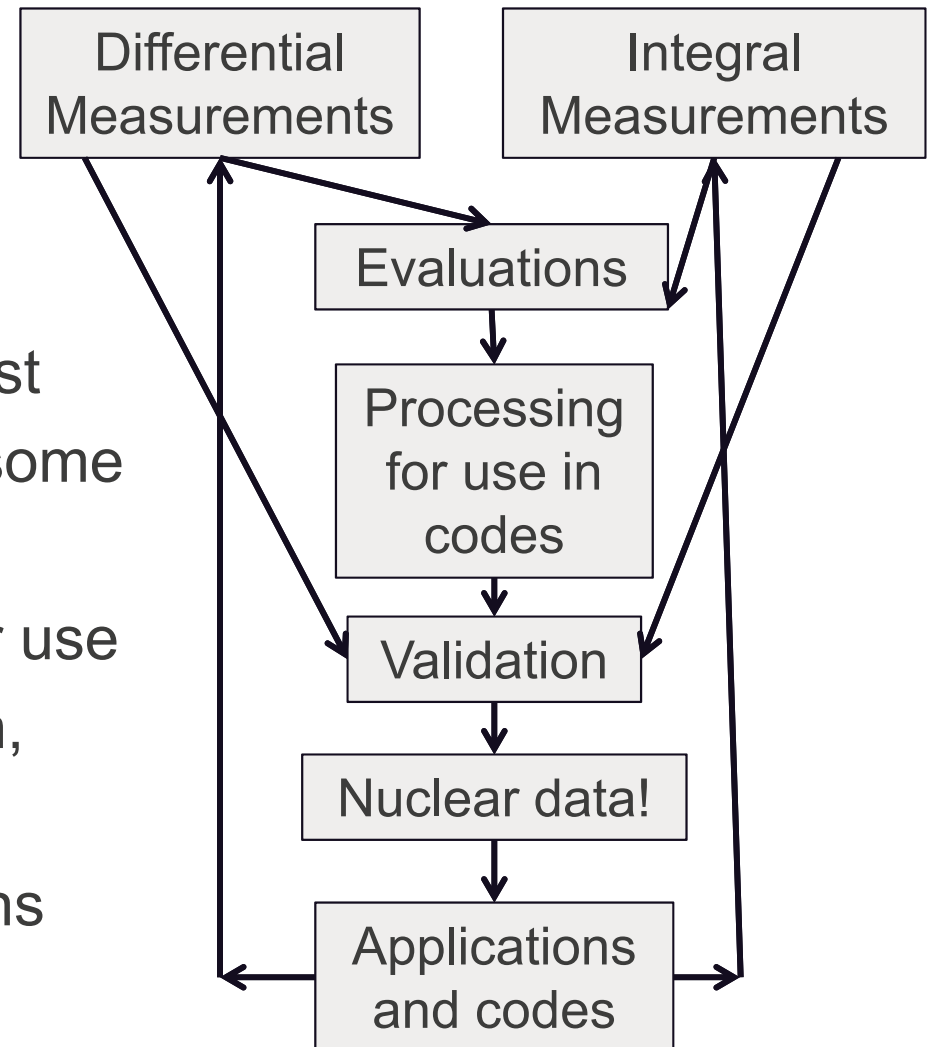
“Life cycle” of nuclear data

- Measurements are made
- Evaluators use those measurements
- Evaluations are processed
- Processed data is validated against integral measurements (and some differential measurements)
- Nuclear data is made available for use



“Life cycle” of nuclear data

- Measurements are made
- Evaluators use those measurements
- Evaluations are processed
- Processed data is validated against integral measurements (and some differential measurements)
- Nuclear data is made available for use
- Users find data that doesn't match, process starts over with new measurements and evaluations



Is there a problem in the nuclear data?

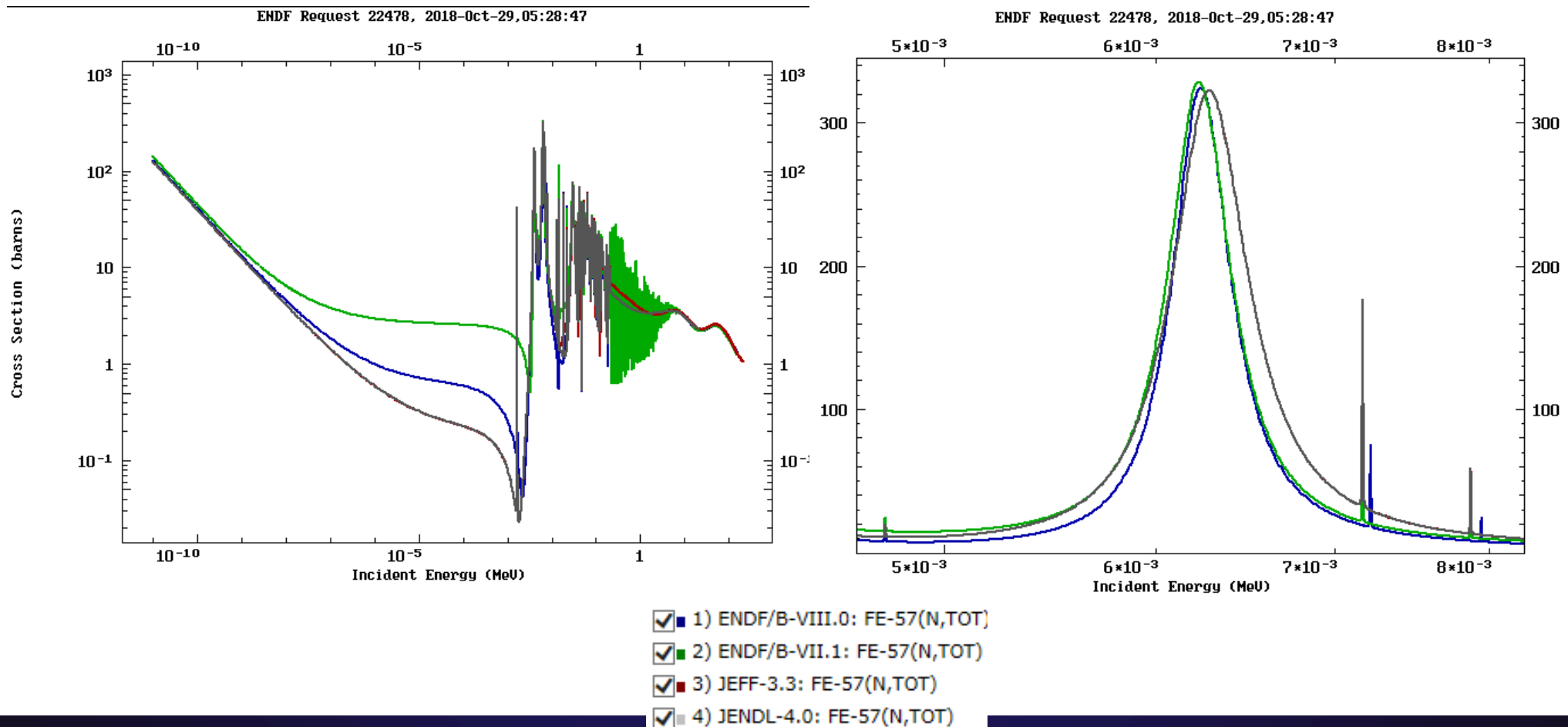
- **Look for indicators of problems**
 - Plot ENDF, JEFF, JENDL - **BNL/NNDC**
 - If they disagree, this might be an indicator of a problem in the nuclear data.
 - If they all agree, this doesn't necessarily mean the nuclear data is good – **many evaluations copy each other!**
 - Plot previous versions of ENDF, JEFF, JENDL
 - Have there been big, recent changes? This might be an indicator of a problem.
 - Have there been no changes in decades? Could be an indicator that little data exists.

Is there a problem in the nuclear data?

- **Think about the whole pipeline**
 - What is the natural abundance of the isotope?
 - This may be an indicator of a lack of measurements – very hard to get isotopic samples
- **Another indicator - measurements**
 - **BNL/NNDC - EXFOR**
 - Sometimes no measurements exist! Also, not all measurements are in EXFOR – and not all data about measurements is in EXFOR
- **Another indicator - Evaluations**
 - Look at header file

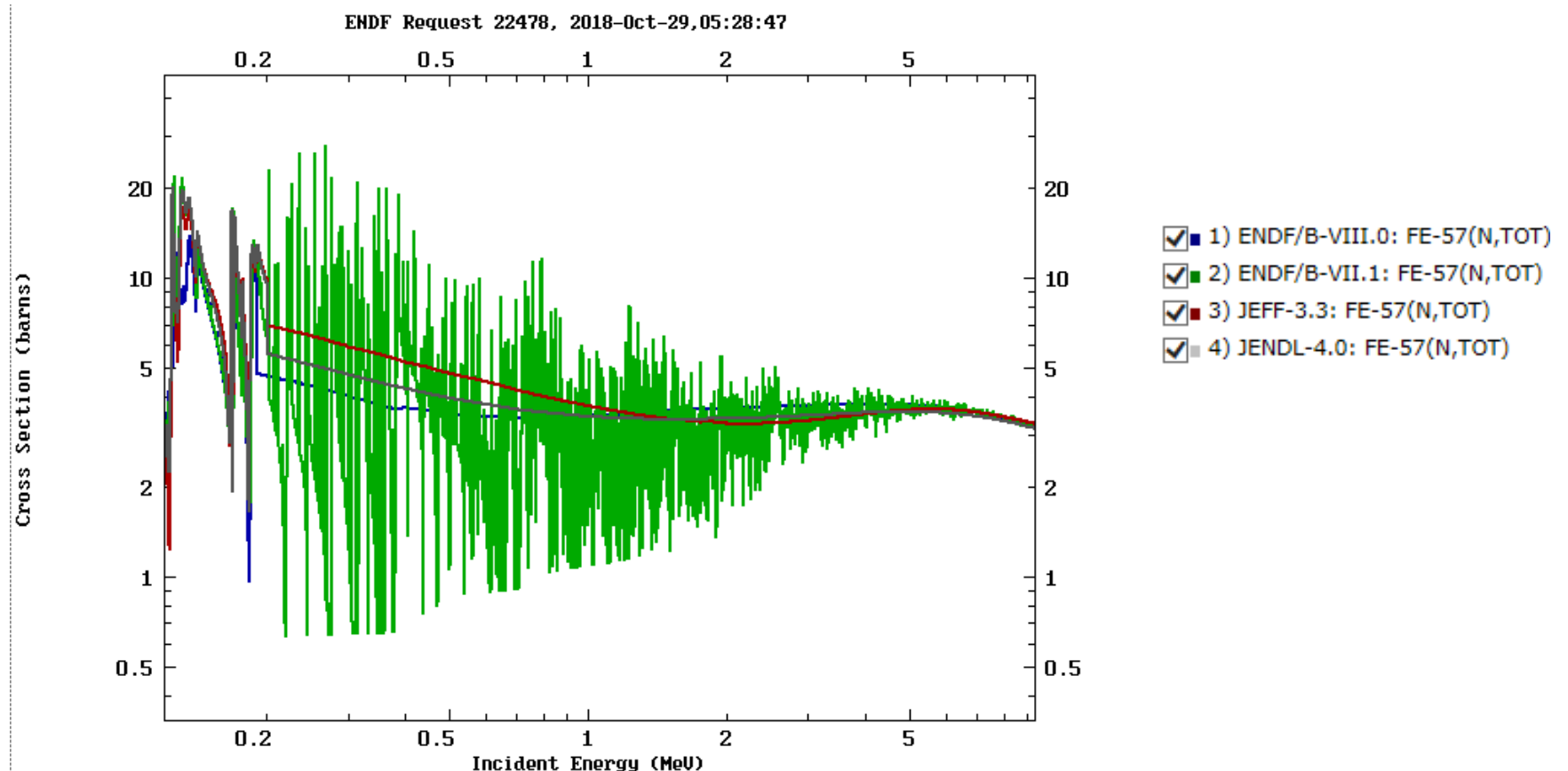
Example – ^{57}Fe – Indicators of nuclear data deficiencies

- Plot ENDF/JEFF/JENDL – n,total
 - Definitely some differences between libraries



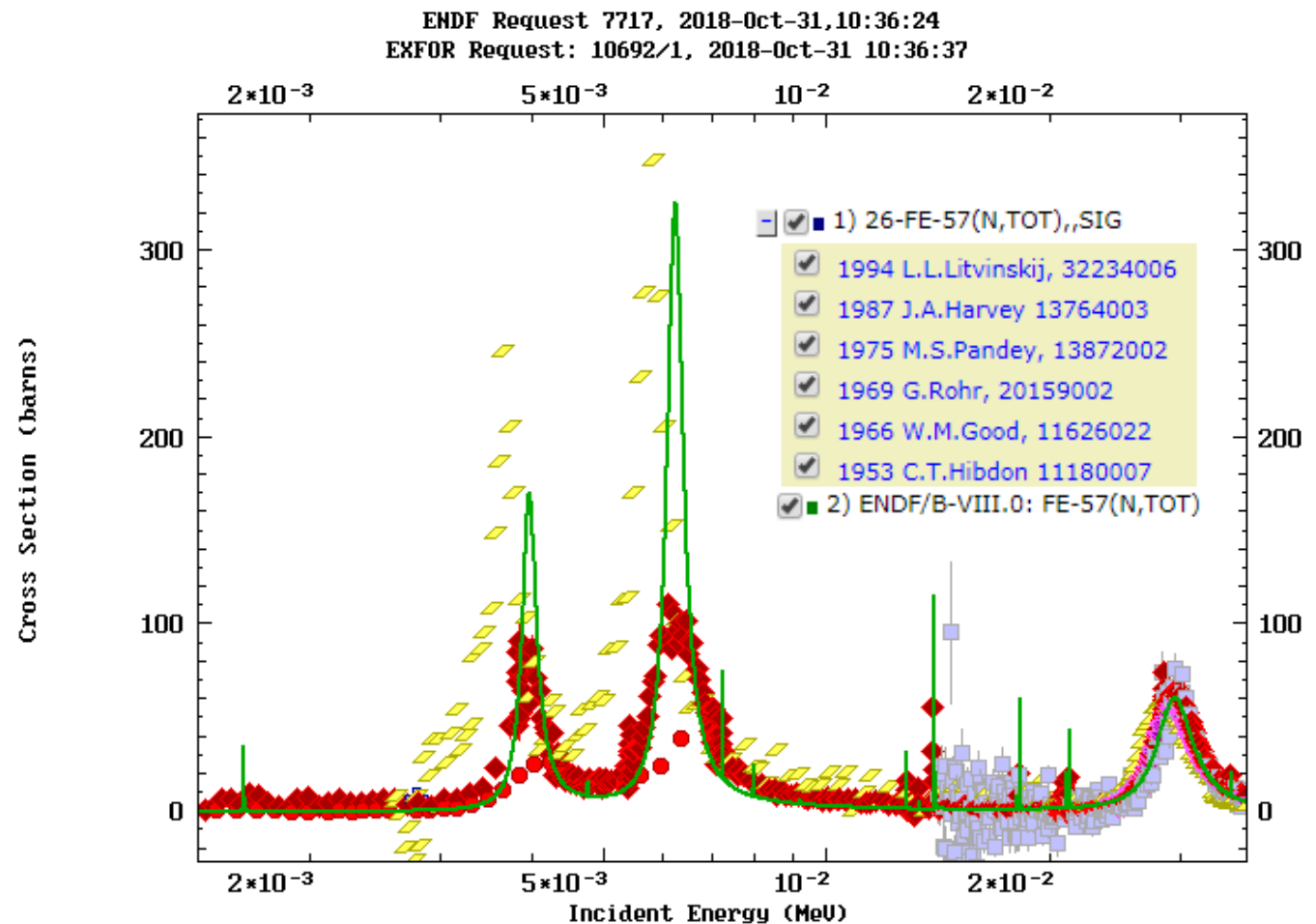
Example – ^{57}Fe – Indicators of nuclear data deficiencies

- Plot ENDF/JEFF/JENDL – n,total
 - Some differences due to evaluation approaches
 - Others due to which measurement data is used



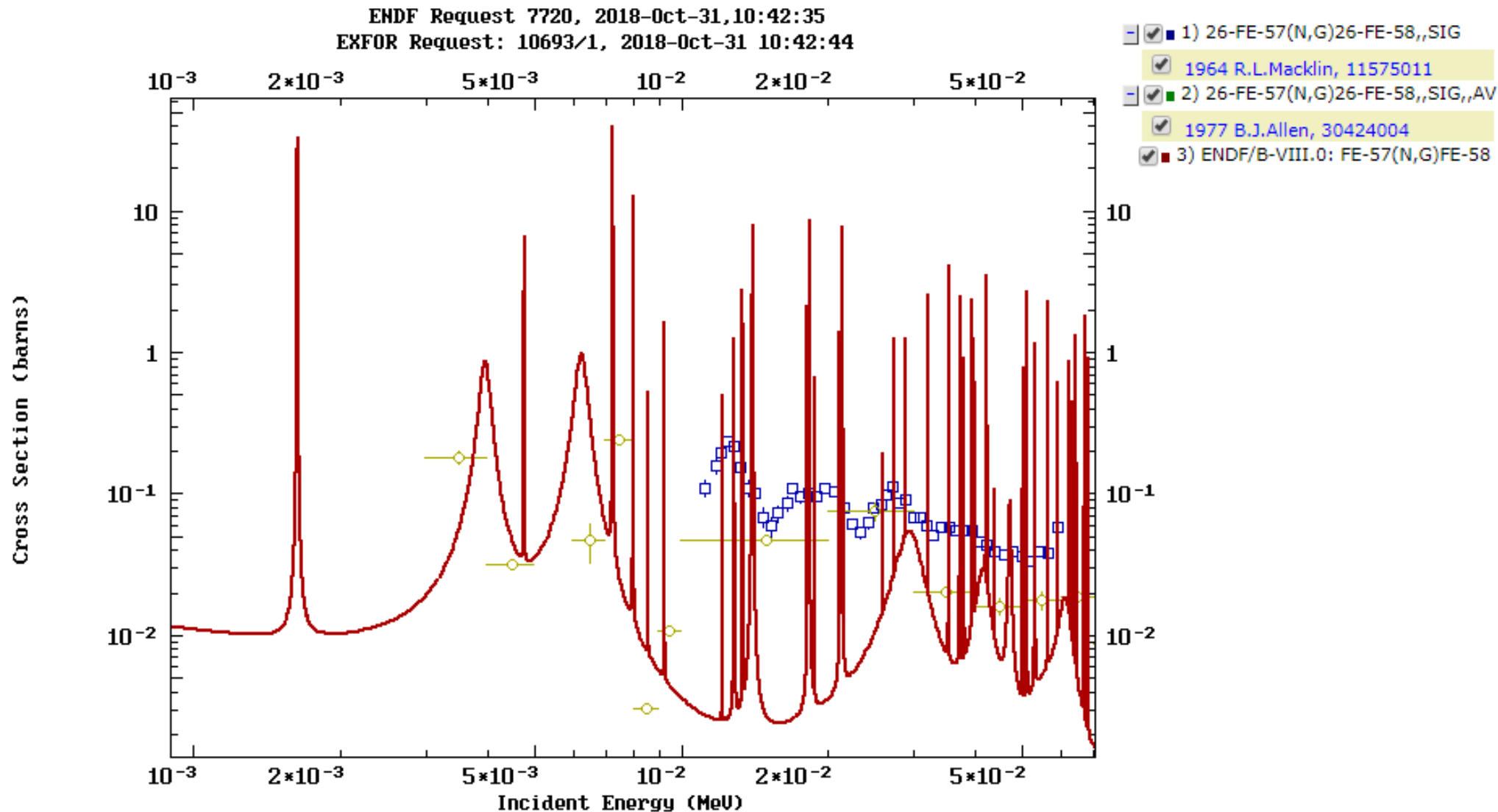
Example – ^{57}Fe – Indicators of nuclear data deficiencies

- ^{57}Fe has a natural abundance of 2.12% - there are probably not many direct measurements of ^{57}Fe .
- Six measurements – 1953, 1966, 1969, 1975, 1987, 1994
- Different measurements with different experimental parameters can be hard to fit together in one evaluation



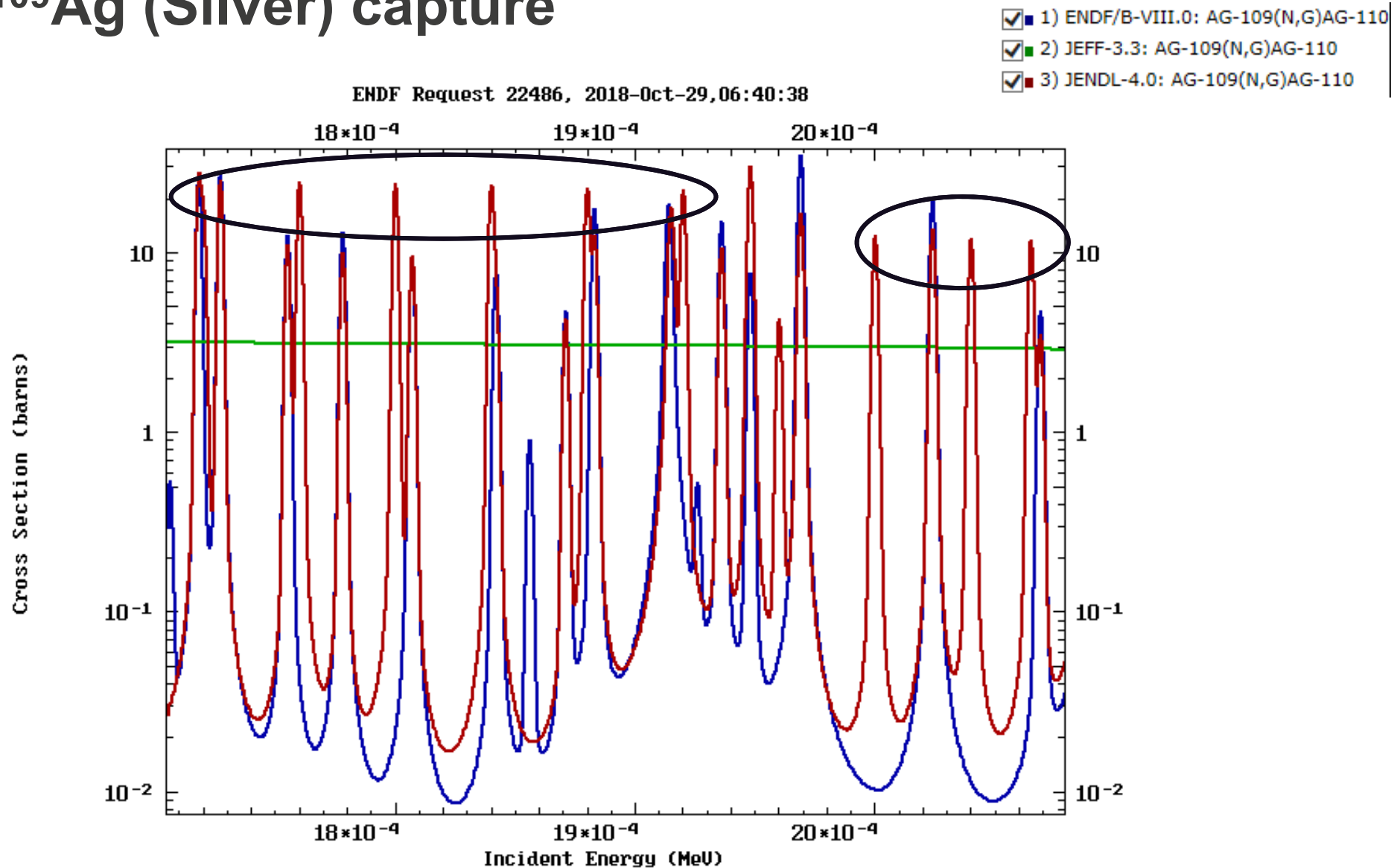
Example – ^{57}Fe – Indicators of nuclear data deficiencies

• What about capture? – Two measurements



Indicators of nuclear data deficiencies – Information in header file

- ^{109}Ag (Silver) capture



Indicators of nuclear data deficiencies – Information in header file

- JENDL-4, resonances were added to better match quasi-integral measurements

MF= 2 Resonance parameters

MT=151 Resolved and unresolved resonances

Resolved resonance parameters (below 7.0095 keV)

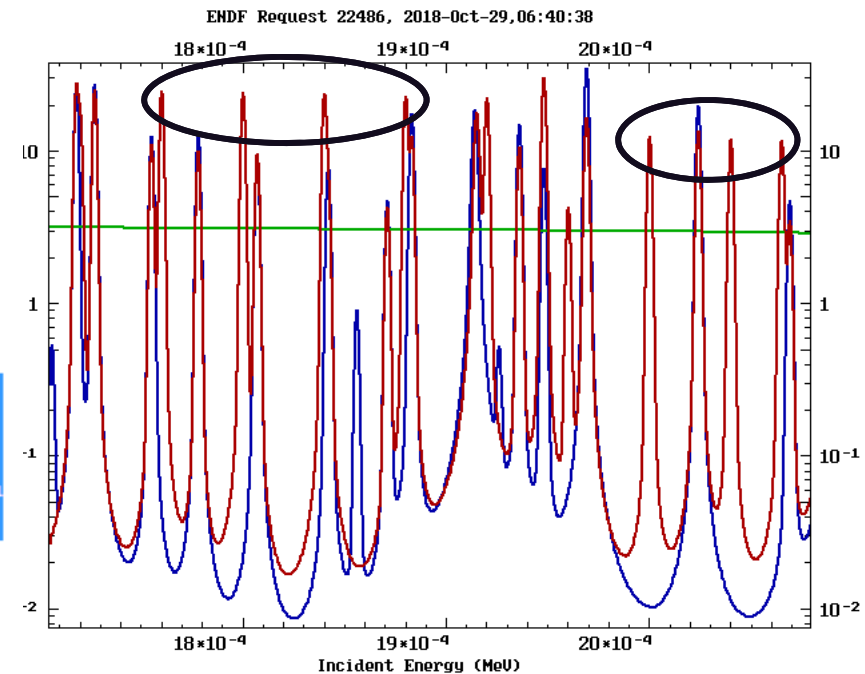
Resolved resonance parameters (below 7.0095 keV) for JENDL-3.3 were based on the experimental data by Moxon and Rae /1/, Garg et al./2/, Asghar et al./3/, Muradjan and Adamchuk /4/, de Barros et al./5/, Pattenden and Jolly /6/, macklin /7/ and Mizumoto et al./8/.

Total spin j and angular momentum l of some resonances were estimated with a random number method and a method of Bollinger and Thomas/9/, respectively.

The capture cross section of JENDL-3.3 between 1.3 and 2.6 keV is too low compared with interpolated values from the lower and higher energy regions. To compensate the lower capture cross section, p-wave resonances with a capture area of 0.02 eV were added every 20 eV between 1.25 and 1.59 keV, and every 40 eV between 1.59 and 2.59 keV. The neutron

width was modified so as to reproduce the capture area measured by Macklin /7/.

In JENDL-4, the data for 5.19 eV - 499.8 eV were replaced with the ones obtained by Lowie et al./10/. A value of 130 meV was used for unknown radiation widths. The neutron width for 264.7 eV was taken from JENDL-3.3. Part of unknown j values were determined by considering the work of Zanini et al./11/. The remaining unknown j values were estimated by a random number method.

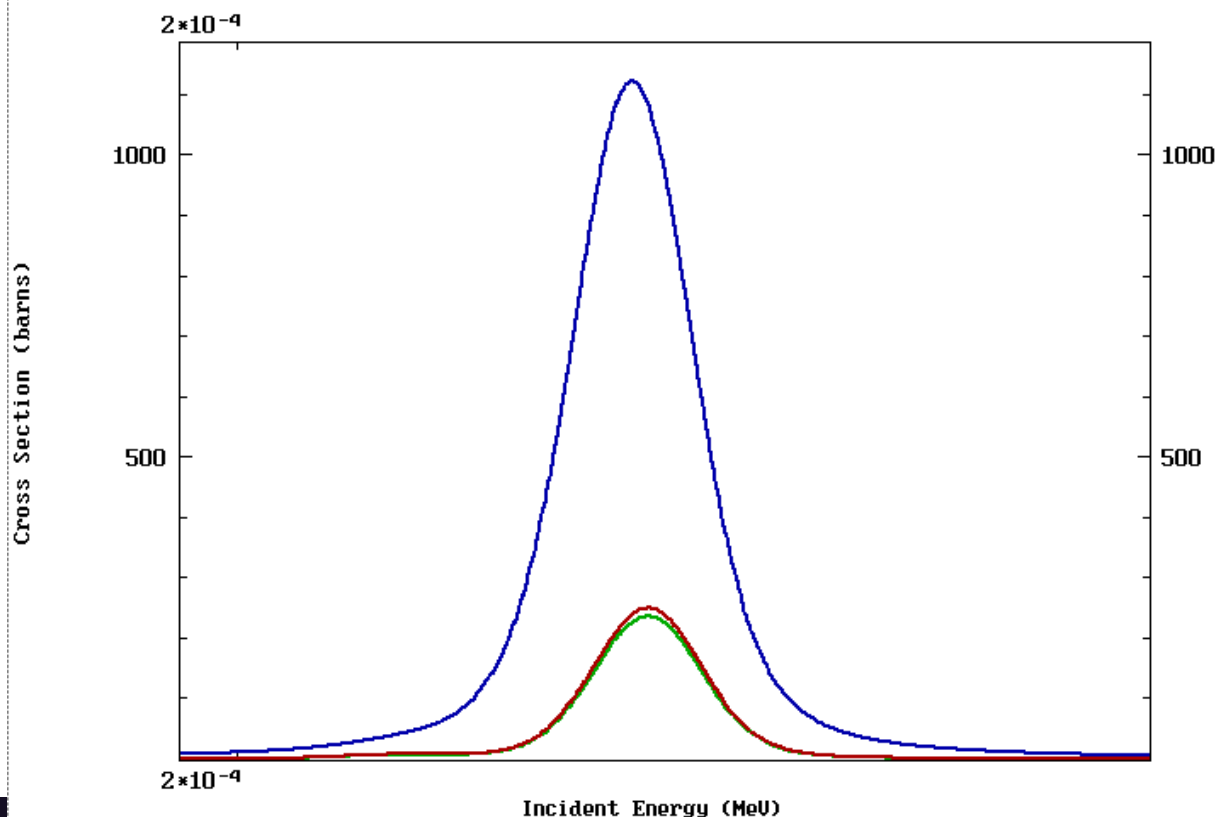


- ✓ 1) ENDF/B-VIII.0: AG-109(N,G)AG-110
- ✓ 2) JEFF-3.3: AG-109(N,G)AG-110
- ✓ 3) JENDL-4.0: AG-109(N,G)AG-110

Indicators of nuclear data deficiencies

- It's also possible that numerical errors exist in the data. 202.5 eV in ^{107}Ag – a resonance parameter is missing a 0 in ENDF (there was a typo). Changes the resonance from ~250 barns to ~2500 barns.

ENDF Request 22489, 2018-Oct-29,08:04:17

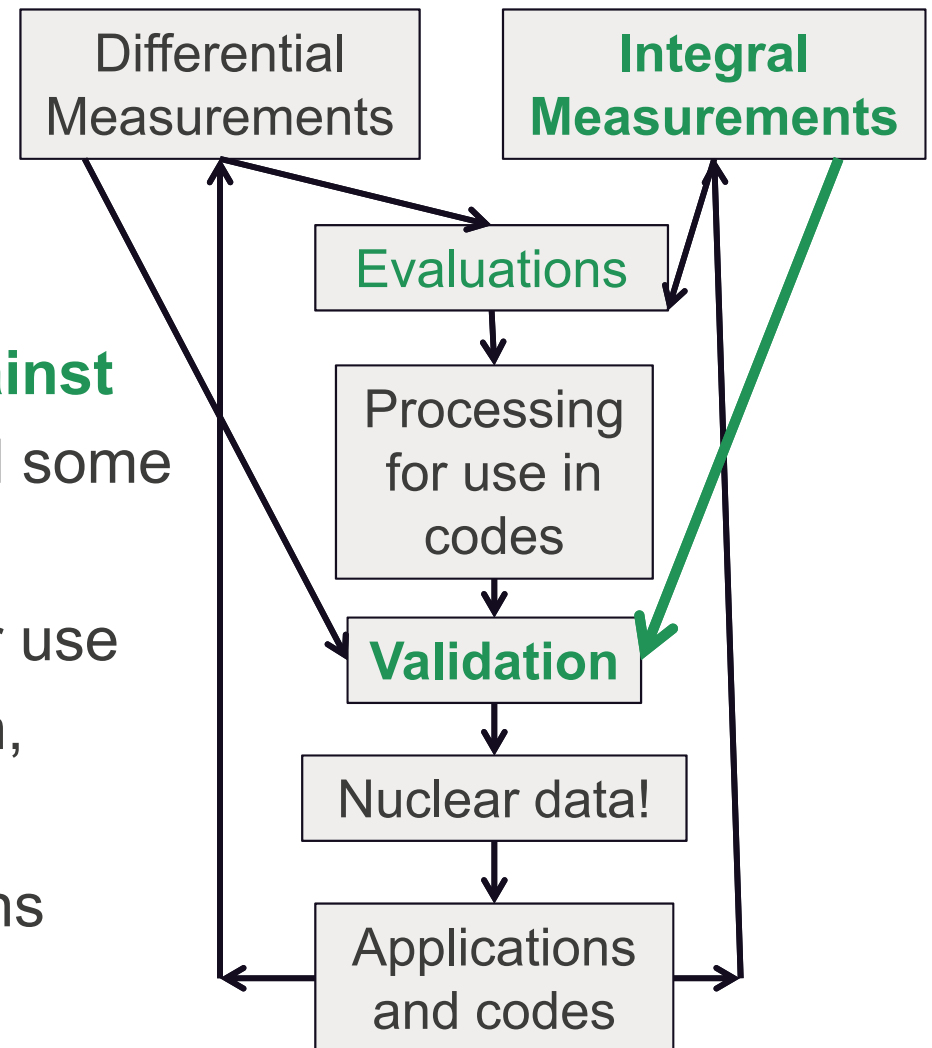


	Energy [eV]	Γ_n (T=300K)
ENDF/B-VIII.0	202.5	0.1793333
JEFF-3.3	202.6	0.01610446
JENDL-4.0	202.6	0.01720000

- 1) ENDF/B-VIII.0: AG-107(N,G)AG-108
- 2) JEFF-3.3: AG-107(N,G)AG-108
- 3) JENDL-4.0: AG-107(N,G)AG-108

What role do Integral Measurements have?

- Measurements are made
- **Evaluators use those measurements**
- Evaluations are processed
- **Processed data is validated against integral measurements** (and some differential measurements)
- Nuclear data is made available for use
- Users find data that doesn't match, process starts over with new measurements and evaluations



What role do Integral Measurements have?

- Evaluations are revised until simulation results can match integral benchmark results
- Integral benchmark (eg. ICSBEP, IRPhEP. LLNL pulsed spheres) are high quality integral measurements that have been thoroughly reviewed and documented
- Example of a plot an evaluator might produce.
- From S.C. van der Marck, “Benchmarking ENDF/B-VII.1, JENDL-4.0, and JEFF-3.1.1 with MCNP6”, 2012

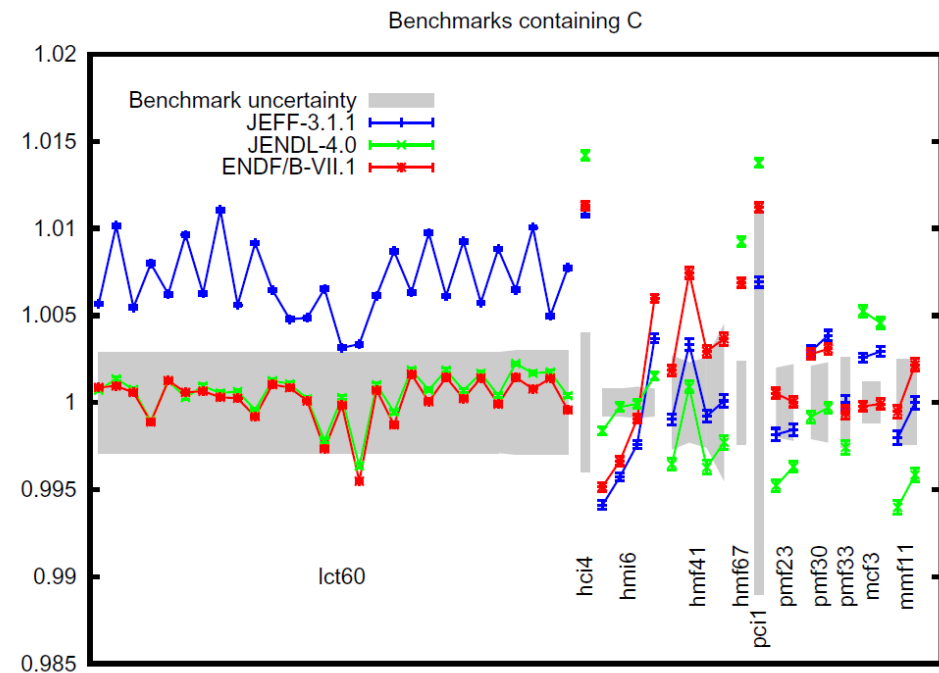


FIG. 22: The results for criticality safety benchmarks containing C, C/E .

What role do Integral Measurements have?

- Lack of benchmarks
 - If there is one benchmark, and the nuclear data matches well, the data still might not be right, because it might have been tuned to match that benchmark!
- Each criticality benchmark also has a range of neutron energies, they are characterized by the energy region where half of the neutrons cause fission
 - Thermal means $> 50\%$ of fissions are below 0.625 eV
 - Fast means $> 50\%$ of fissions are above 100 keV
 - Intermediate means $> 50\%$ of fissions fall between 0.625 eV and 100 keV
 - Mixed means no energy region has $> 50\%$ of fissions

What role do Integral Measurements have?

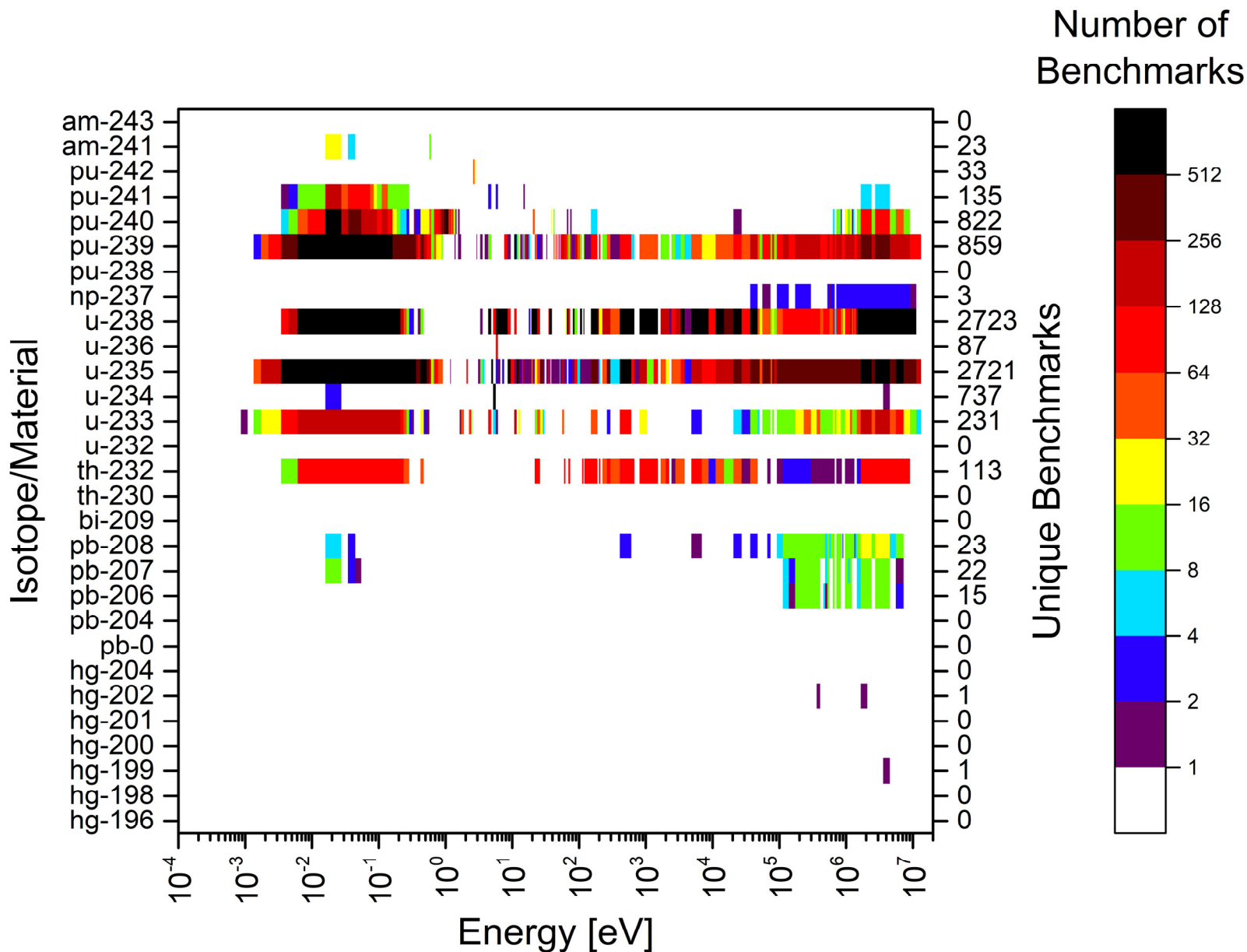
- To review – integral benchmarks are used in evaluations and used to validate nuclear data
- Some materials have many benchmarks, some only have a few
- Different benchmarks have different sensitivities to materials, and are more/less sensitive to different energies
- **How do you find deficiencies in integral benchmarks? What is missing?**

Our Approach

- **Look at all benchmarks, all isotopes/materials, all interactions, all energies**
- **Use sensitivity files to determine where gaps exist**
 - Sensitivity is $(dk_{\text{eff}}/k_{\text{eff}})/(d\sigma/\sigma)$ – change in k_{eff} for a change in cross section
 - 85% of configurations have sensitivity data from NEA
- **Distill data down to a readable form**
 - Heatmaps
- **Next slide – Heatmap of the number of benchmarks that have a sensitivity $> 10^{-3}$ for each energy (238 groups), for each isotope/material**

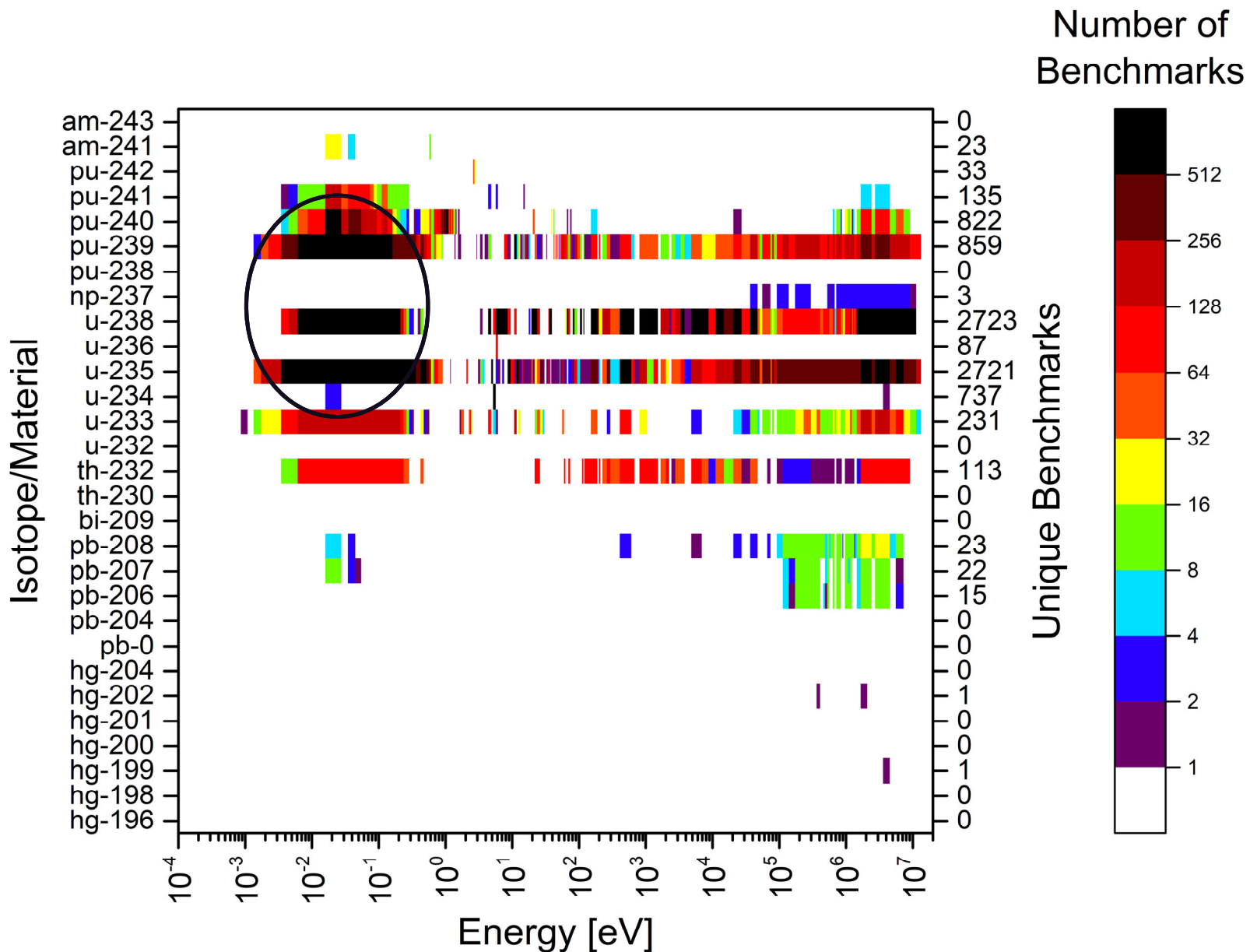
Integral Benchmark Heatmaps

- Each line is an energy bin
- Each color is how many benchmarks are sensitive to the total cross section of that energy bin of that isotope
- Can do the same for scattering, capture, fission, even nubar



Integral Benchmark Heatmaps

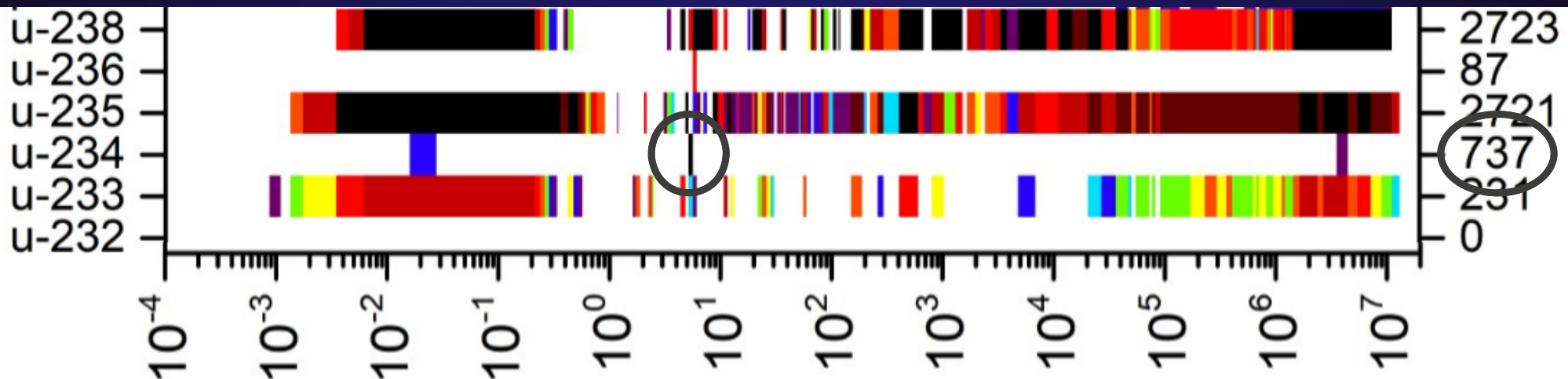
- Some things are very easy to see – Lots of benchmarks sensitive to ^{235}U and ^{239}Pu
- But there is much more information to glean from this



Sensitivities

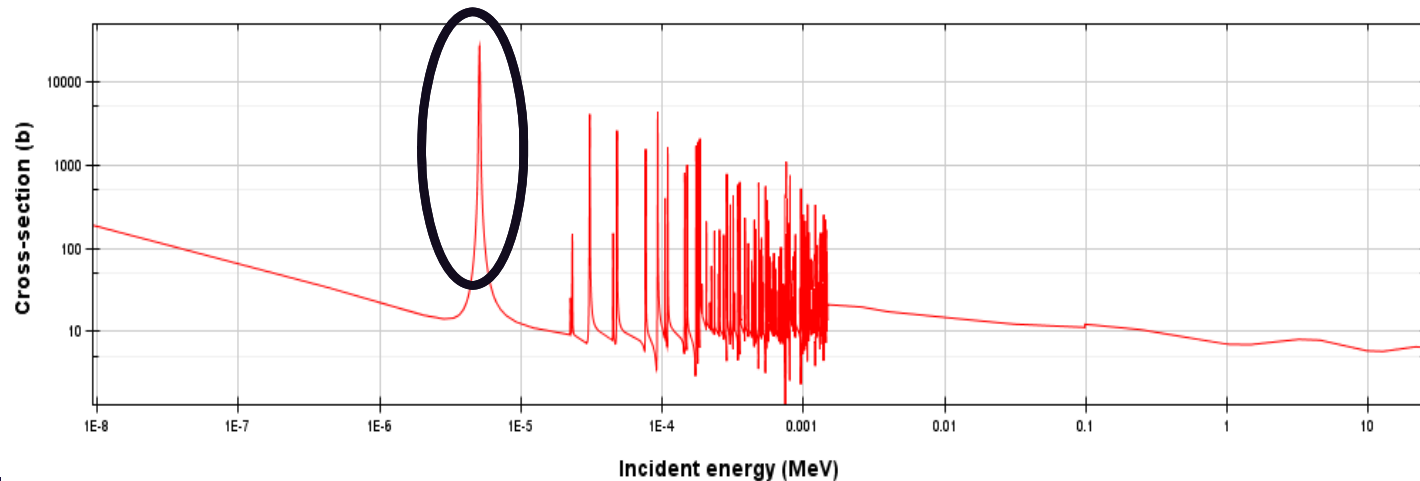
- **Sensitivities are impacted by many factors and all are convoluted together**
 - Cross section – if the cross section is high, then a small % change in cross section has a high impact on k_{eff} /sensitivity
 - Amount of the material in the system and Isotopic Abundance – if isotopic abundance is higher, then sensitivity will be higher
 - Flux – thermal systems are very sensitive to thermal cross sections
- **One asterisk**
 - These plots are looking at sensitivity to total cross section, in many cases, one interaction can have a positive impact on k_{eff} , while another has a negative impact on k_{eff} . Perfect example is thermal ^{235}U – cross sections for capture and fission are both high (in the low eV region, some capture resonances are higher than fission). Because of this, the sensitivity to total cross section can actually be quite low, even when sensitivities to capture/fission are high, because they are canceling each other out.

Sensitivities – Cross Sections



- Same plot as before – zoomed in on isotopes of uranium
- Look at ^{234}U
 - 737 benchmarks are sensitive to it, but only at one energy bin, 5-5.4 eV
 - ^{234}U has a ~26000 barn resonance at 5.16 eV (mostly capture)

Incident neutron data / ENDF/B-VII.1 / U234 / MT=1 : (n,total) / Cross section

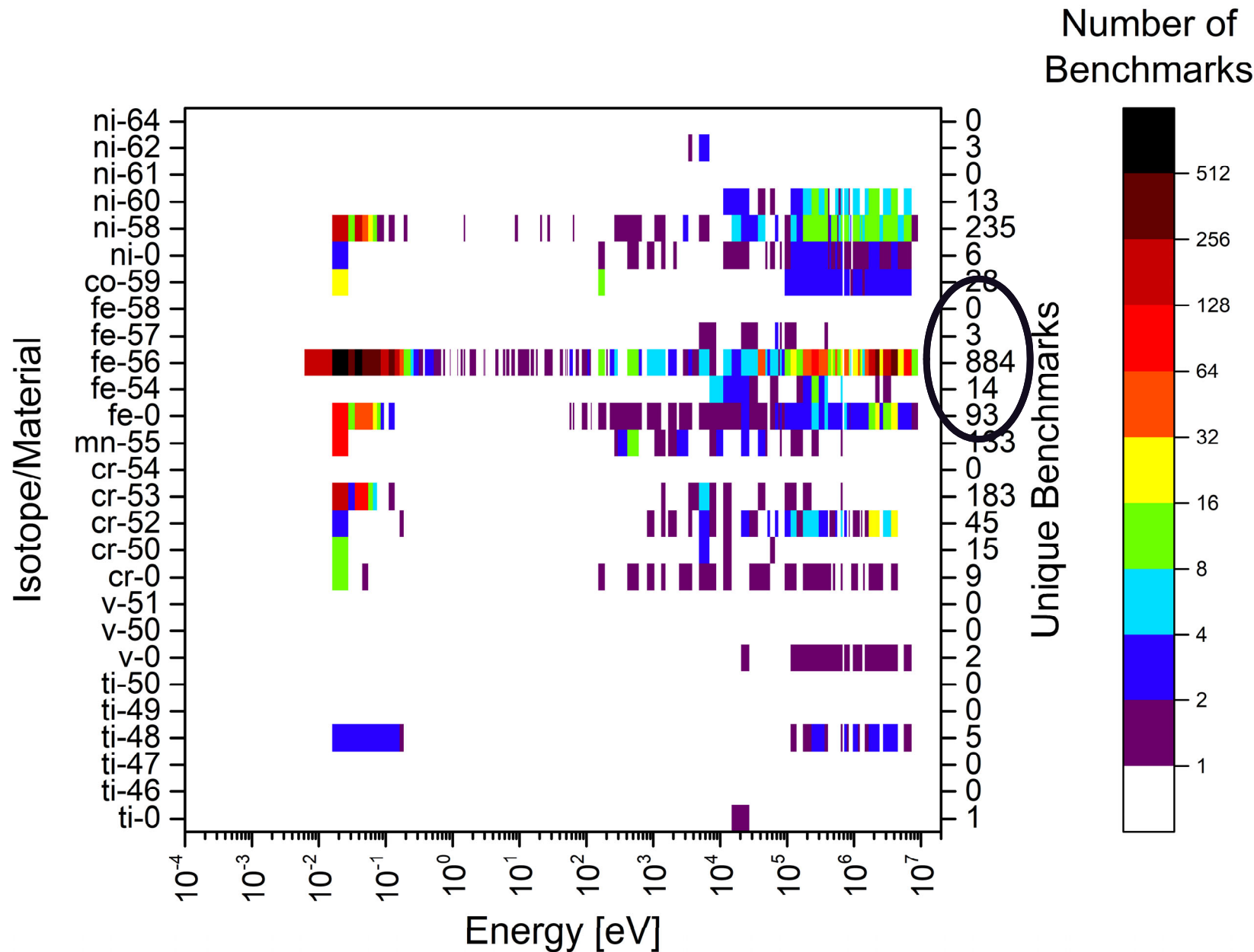


Sensitivities – Isotopic Abundance

-One example is iron (Fe)

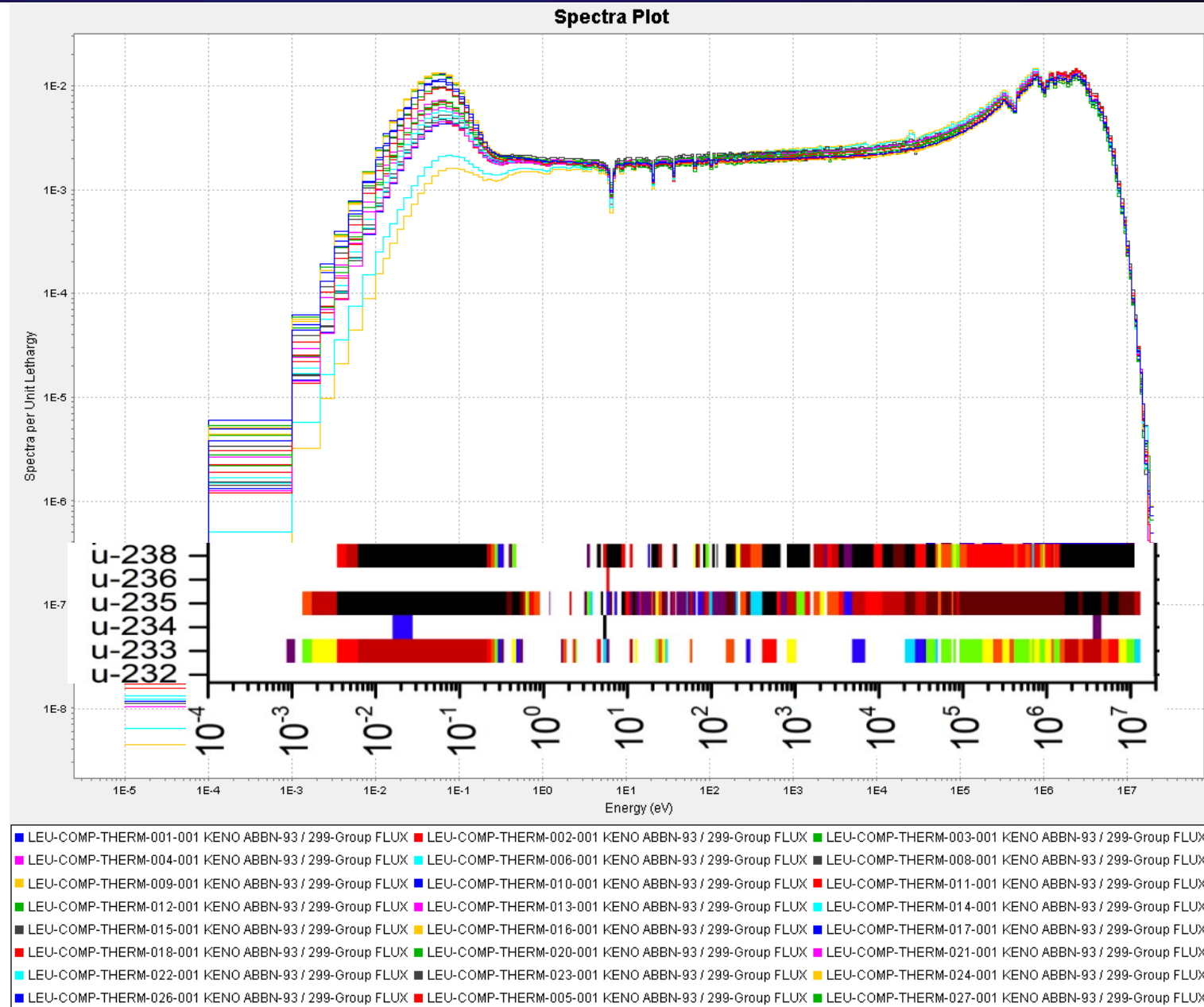
-91.75% of iron is ^{56}Fe

-Many benchmarks are sensitive to iron, but very few are sensitive to ^{54}Fe (5.85%), ^{57}Fe (2.12%), and ^{58}Fe (0.28%).



Sensitivities - Flux

- Many benchmarks (~1200/4000) are LCT – Low enriched, compound, thermal
- Fluxes for just 28 of them – most look pretty similar
- They also look similar to the ^{235}U and ^{238}U sensitivities - more flux means higher sensitivity

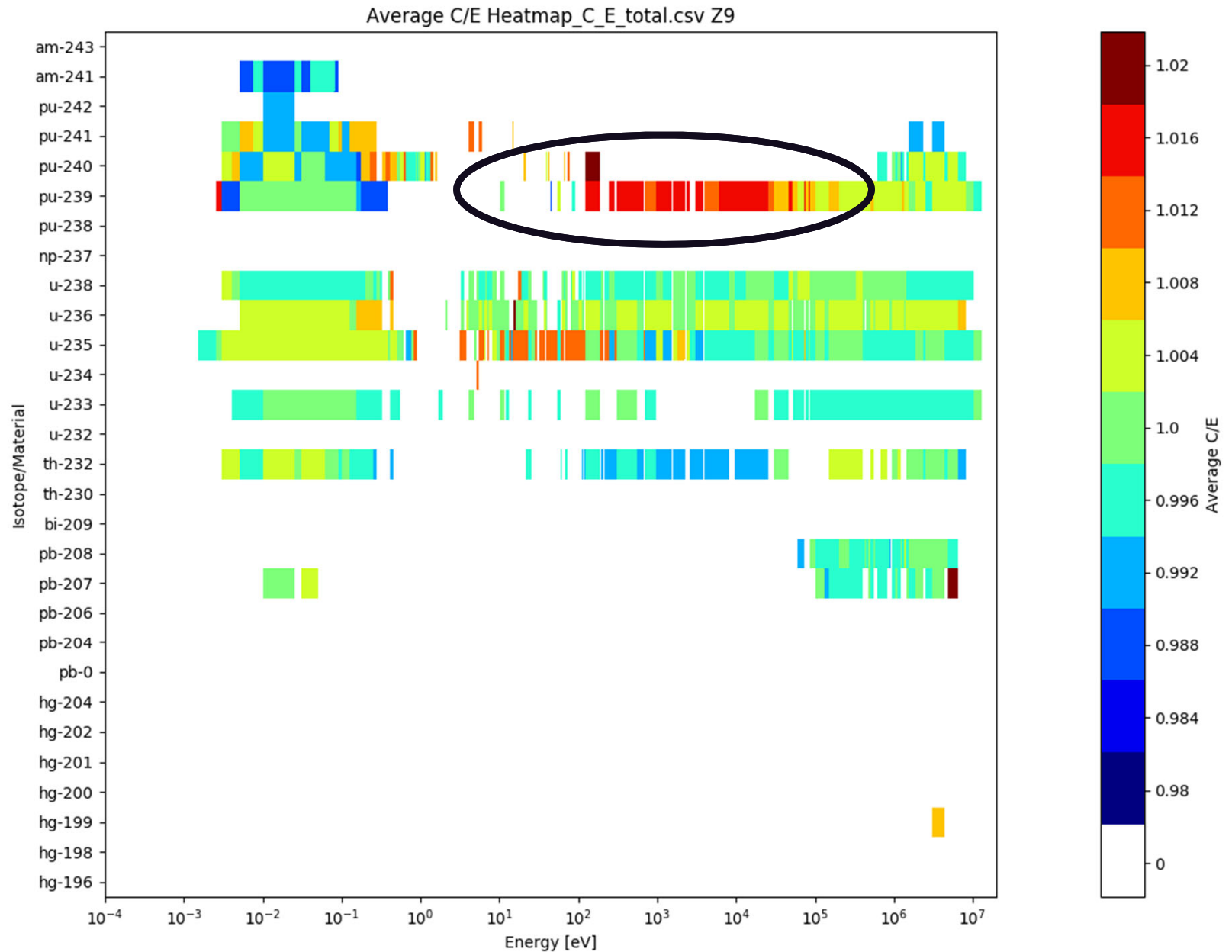


Let's go a little deeper

- **Number of benchmarks is good, but doesn't tell the whole story**
- **How well are those benchmarks simulated by MCNP?**
 - van der Marck ran those simulations for ENDF/B-VII.1, JENDL-4.0, and JEFF-3.1.1
- **Next set of heatmaps – Average C/E**
 - MCNP6 simulation using ENDF/B-VII.1 cross sections
 - $C = \text{Simulation } k_{\text{eff}}$; $E = \text{Experimental } k_{\text{eff}}$
 - Each bin is the average C/E for the benchmarks that energy bin is sensitive to
 - Example – if the HMF-60-1, ICT-1-8, LCT-33-2 benchmarks are sensitive to ^{19}F in the 1 MeV energy bin, calculate the average C/E for those 3 benchmarks

Average C/E Heatmaps

^{239}Pu has an average C/E well above 1 from ~100 eV to 100 keV

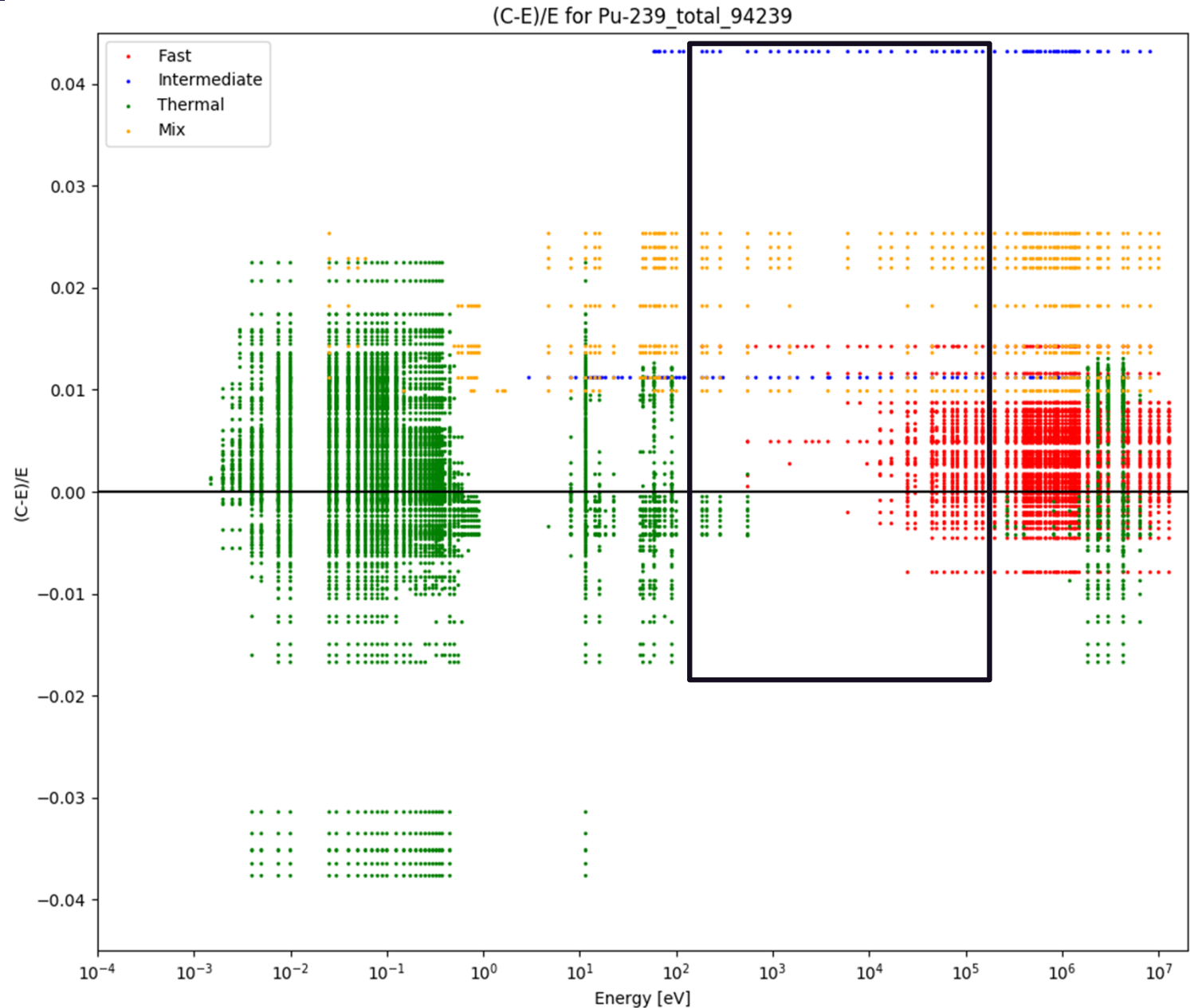


(C-E)/E Distribution for ^{239}Pu

In that energy region, nearly all benchmarks have a (C-E)/E above 0.

Interestingly, all intermediate or mixed spectrum benchmarks are above 0.

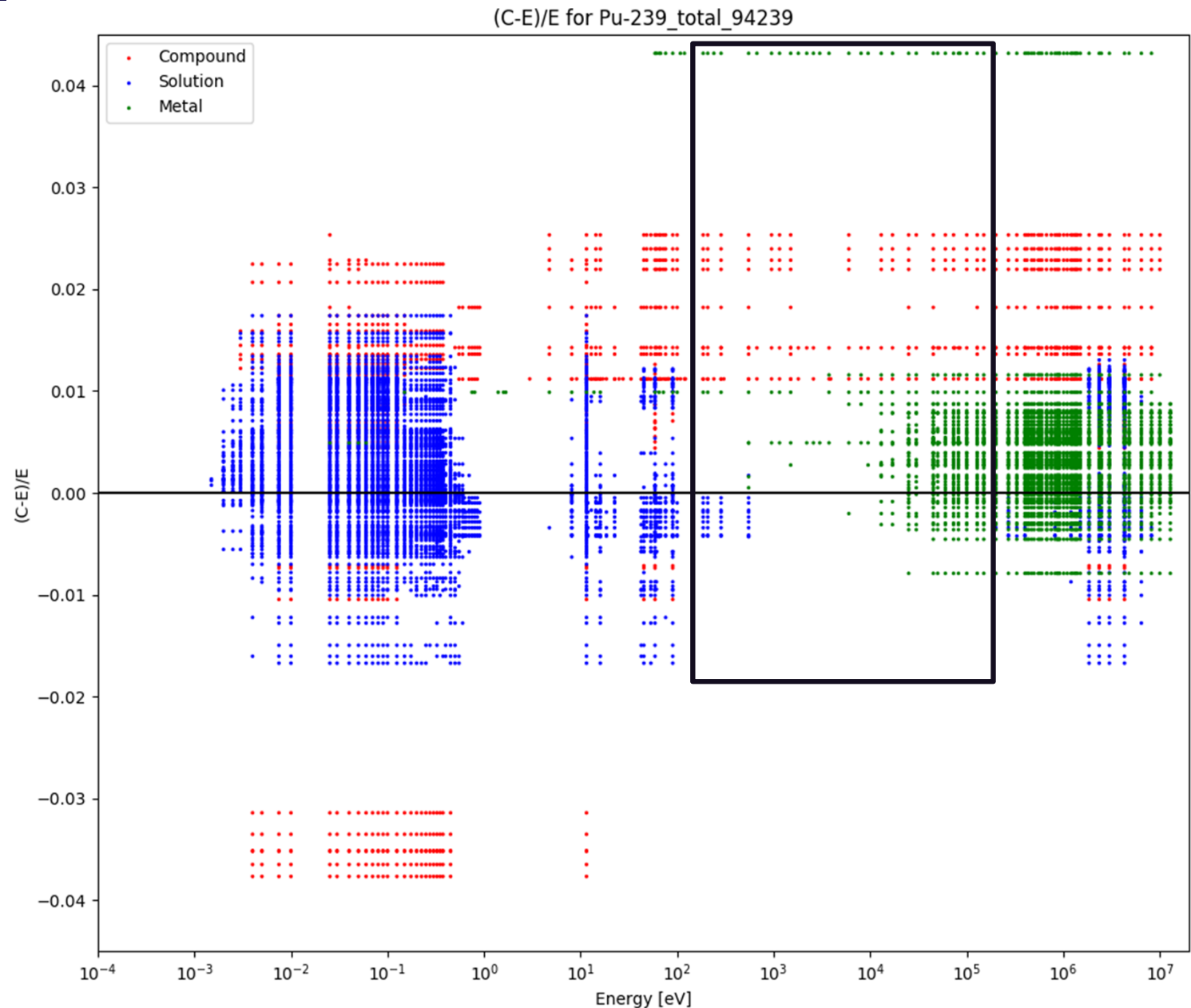
Might be worth reviewing these benchmarks and making new intermediate ^{239}Pu benchmarks.



(C-E)/E Distribution for ^{239}Pu

Plots can also be created with different color schemes:

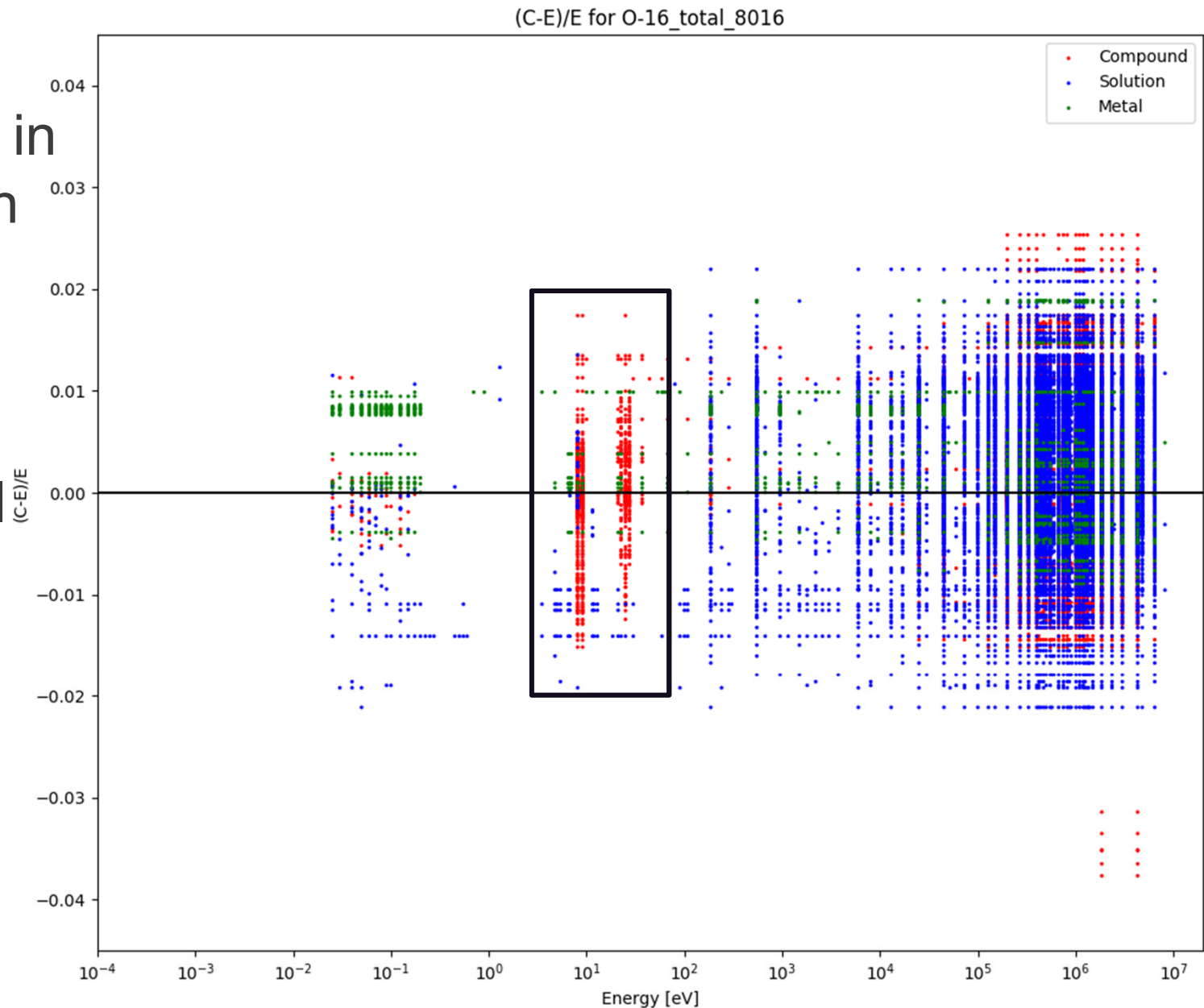
- Fuel type (compound, metal solution)
- Fuel enrichment (HEU, IEU, LEU, Pu, Mixed)
- Energy region (Fast, Thermal, Intermediate, Mixed)
- Sensitivity



(C-E)/E Distribution for ^{16}O

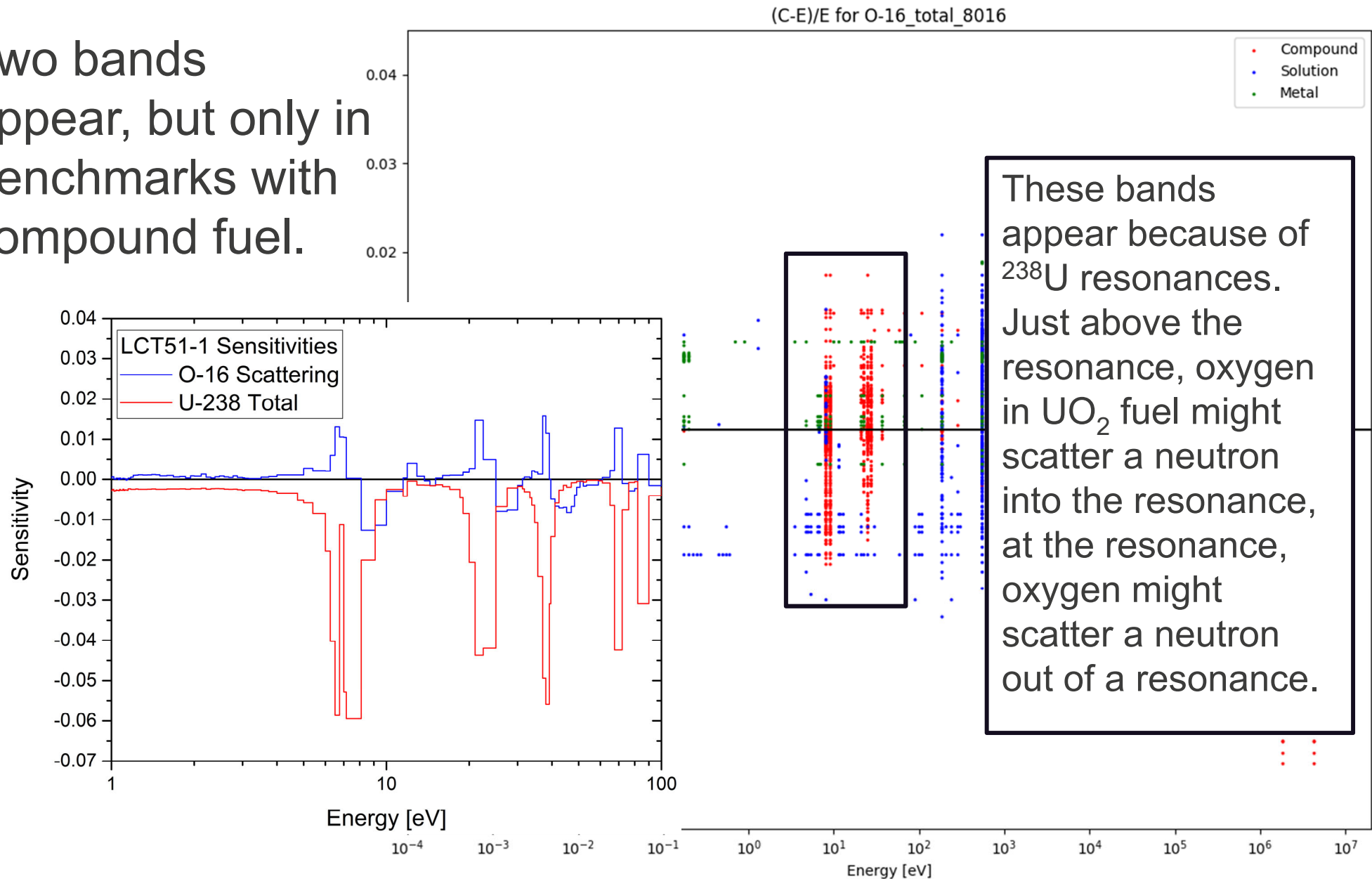
Two bands appear, but only in benchmarks with compound fuel.

Oxygen has no resonances until 430 keV.



(C-E)/E Distribution for ^{16}O

Two bands appear, but only in benchmarks with compound fuel.



Review

- There are many indicators of nuclear data deficiencies
- Integral benchmarks are important for validating nuclear data
 - Lack of benchmarks may be an indicator that nuclear data has issues
- These heatmaps helps to create an easy way to determine what benchmarks are sensitive to a material in a particular energy region – and helps to find materials/energy regions with few or no benchmarks
- Even if benchmarks exist, simulations may not agree with the benchmarks due to issues in nuclear data – average C/E plots and individual C/E plots can help to find those discrepancies – for all energy regions

Review

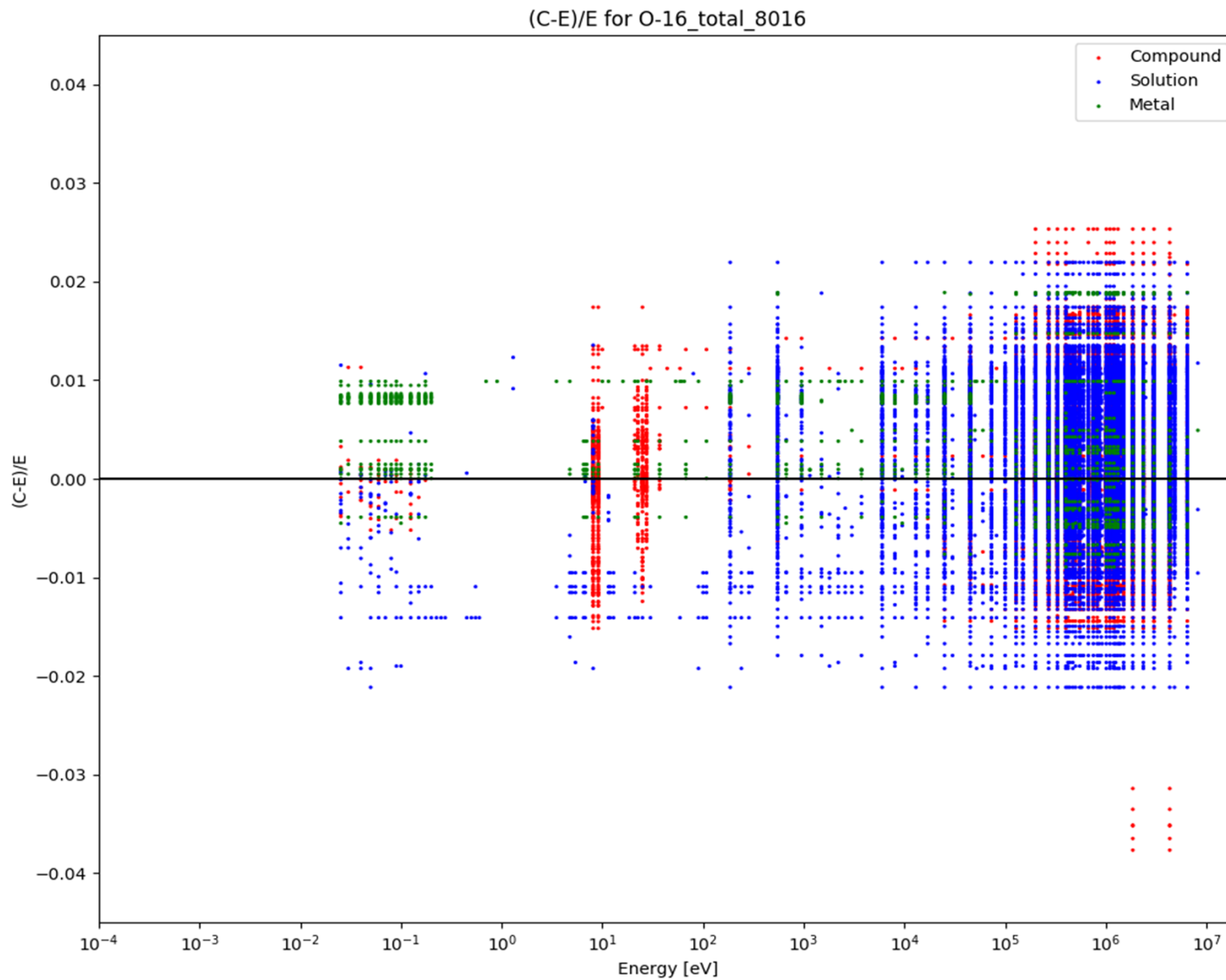
- **These plots/data will be useful to:**
 - Members of the nuclear community trying to determine if there are problems in nuclear data
 - Integral experimenters trying to determine where gaps exist so they can produce useful benchmarks
 - Differential experimenters and evaluators looking for materials/energy regions where nuclear data does not match benchmarks so they can best focus their efforts

Next Steps

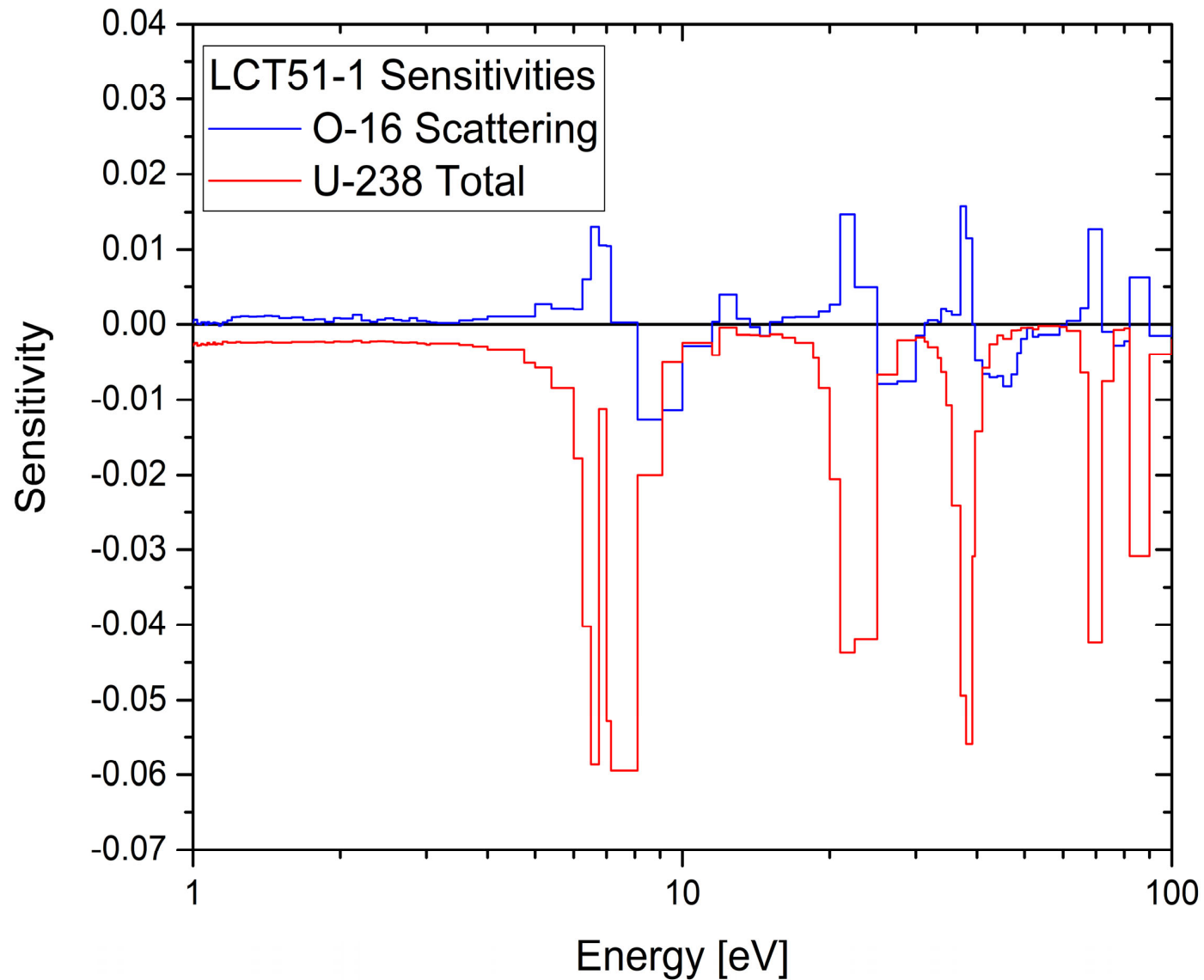
- **Refine results and find other interesting results**
- **Simulate all benchmarks with MCNP6.2, ENDF/B-VIII.0 to get most up to date C/E results**
- **Application Specific results**
 - Find where gaps are, what measurements would add the most value
 - Take into account flux and cross section
- **Thanks for listening!**

Appendix A – Heatmaps, Number of Benchmarks

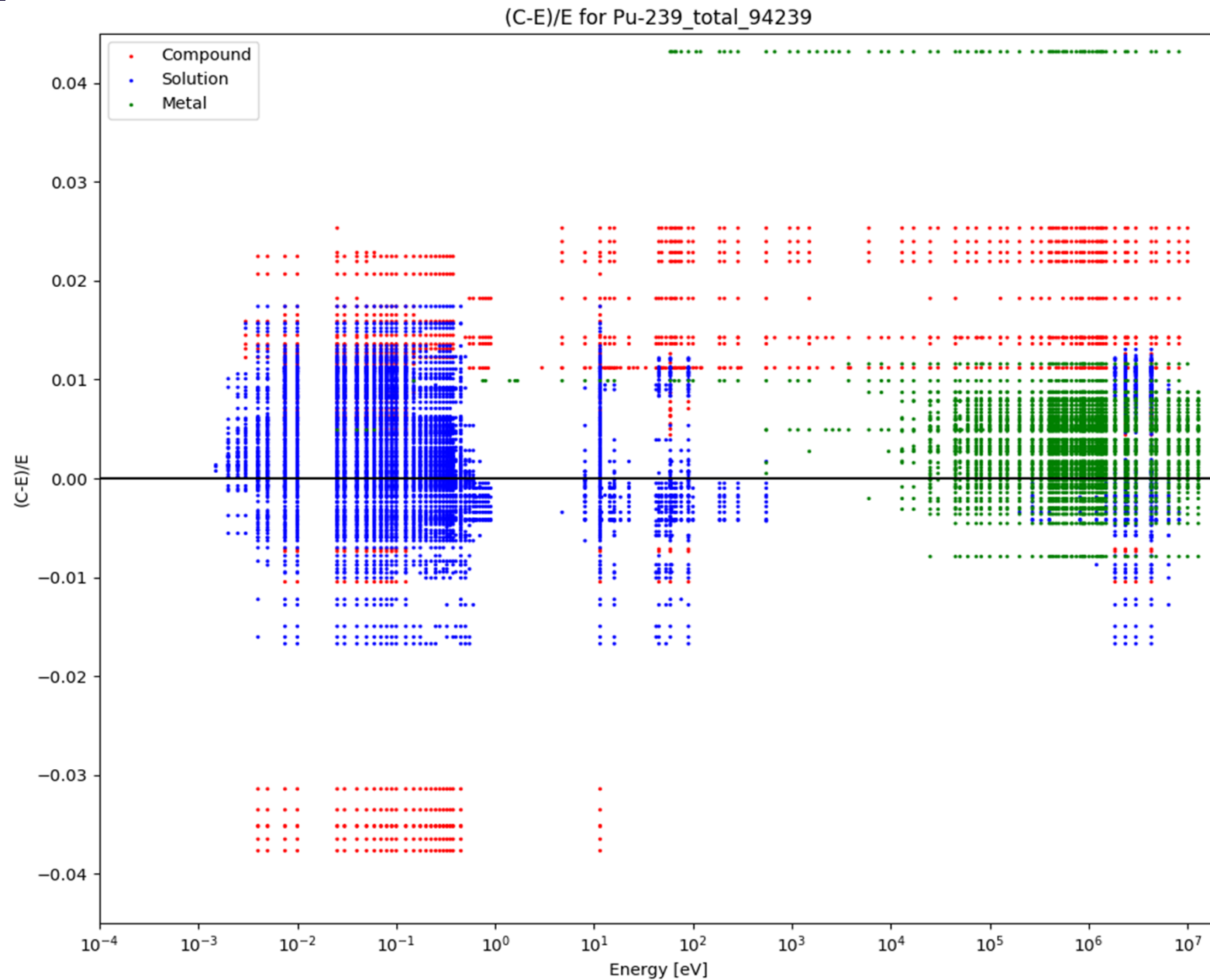
$(C-E)/E$ for O-16 total



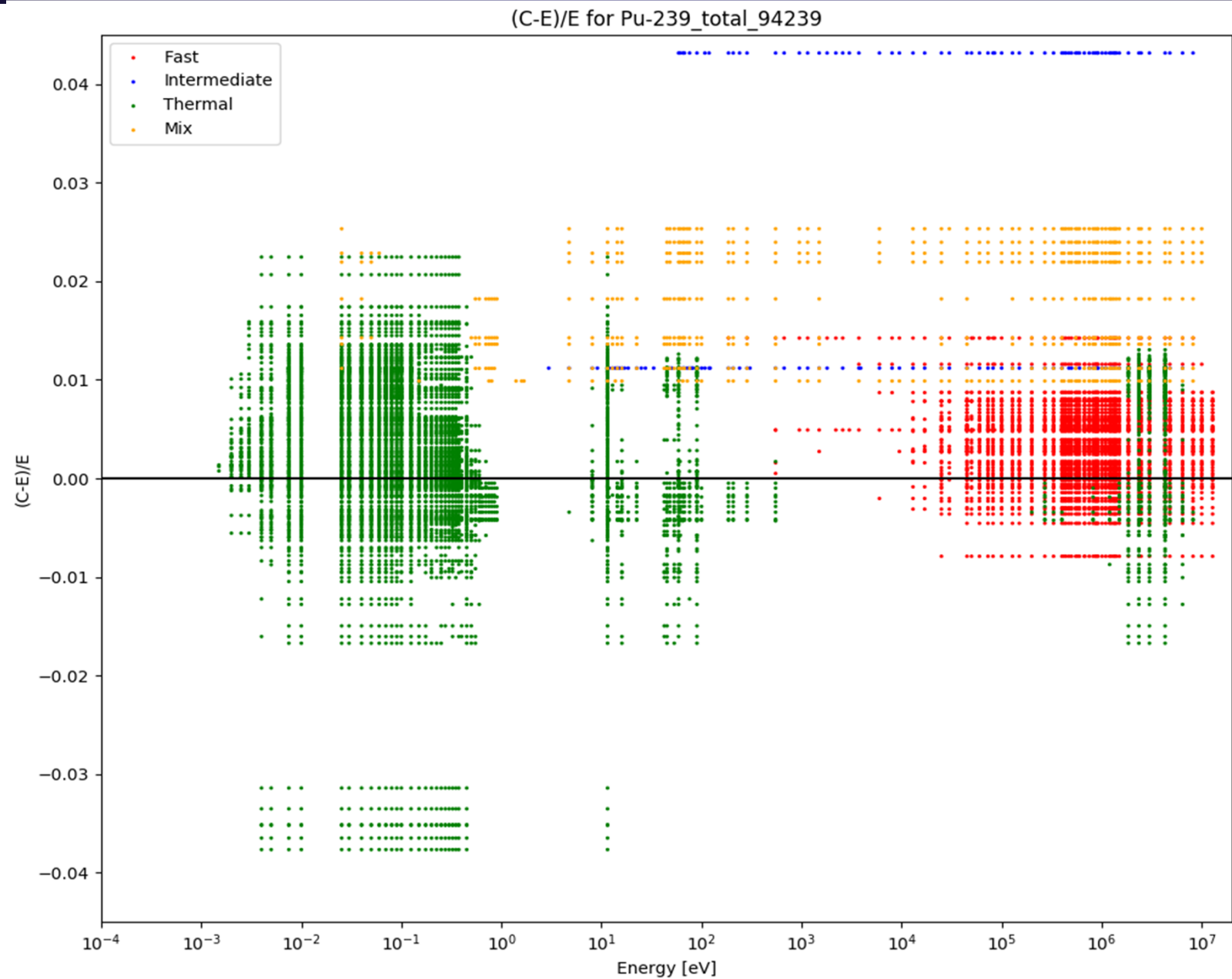
LCT51-1 Sensitivities – O-16 scattering and U-238 total



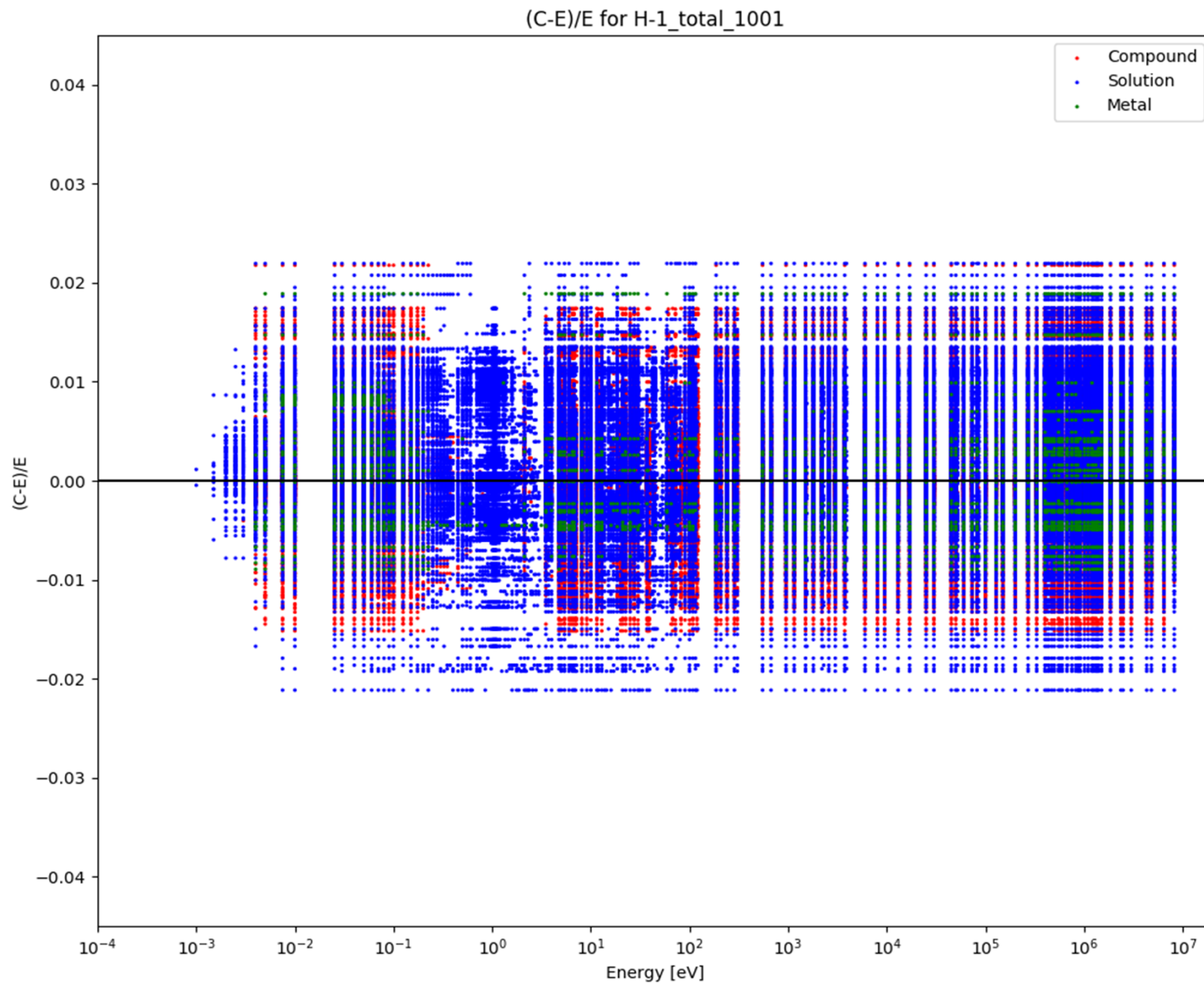
$(C-E)/E$ for Pu-239 total – colored by fuel type



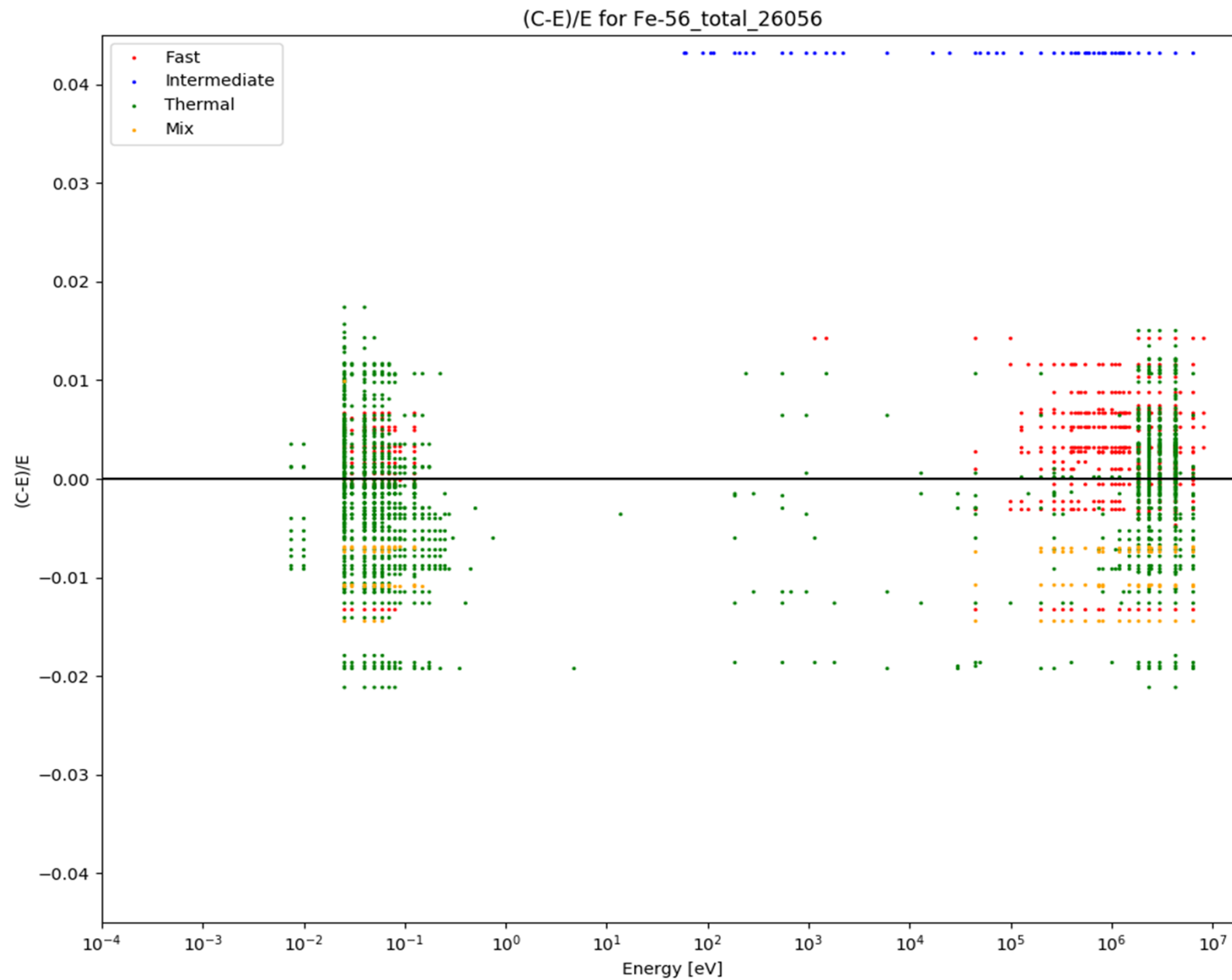
$(C-E)/E$ for Pu-239 total – colored by energy



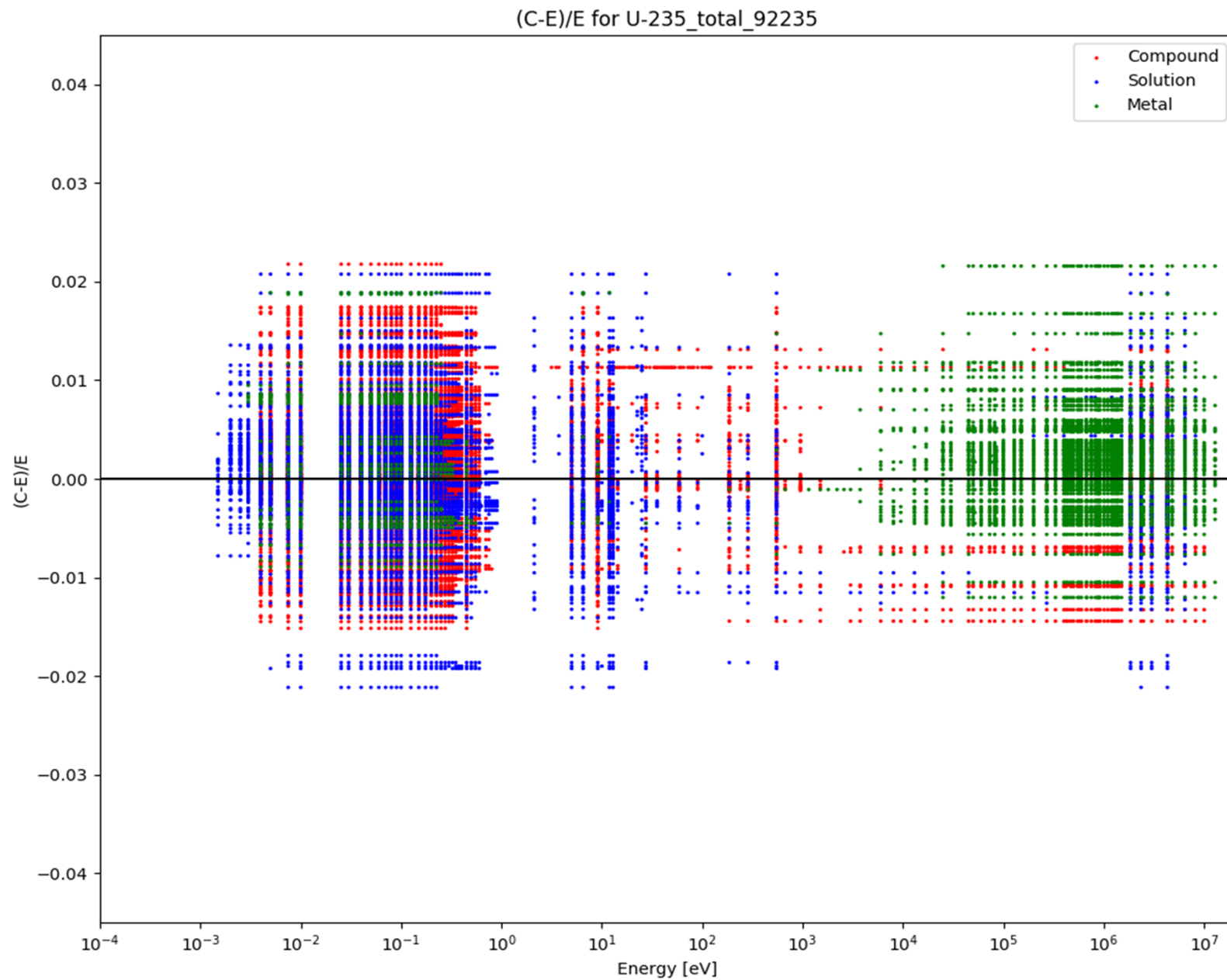
$(C-E)/E$ for H-1 total



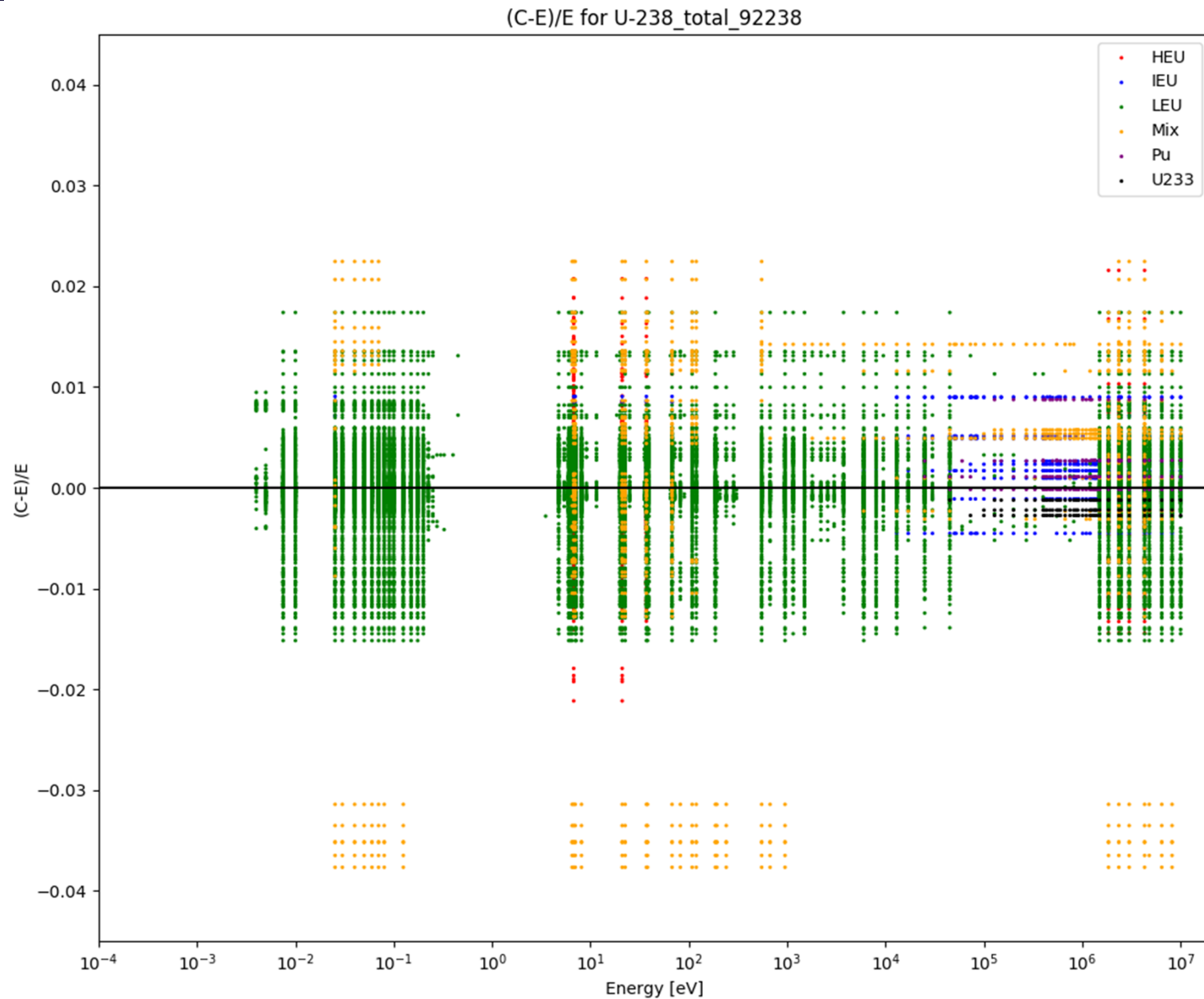
$(C-E)/E$ for Fe-56 total



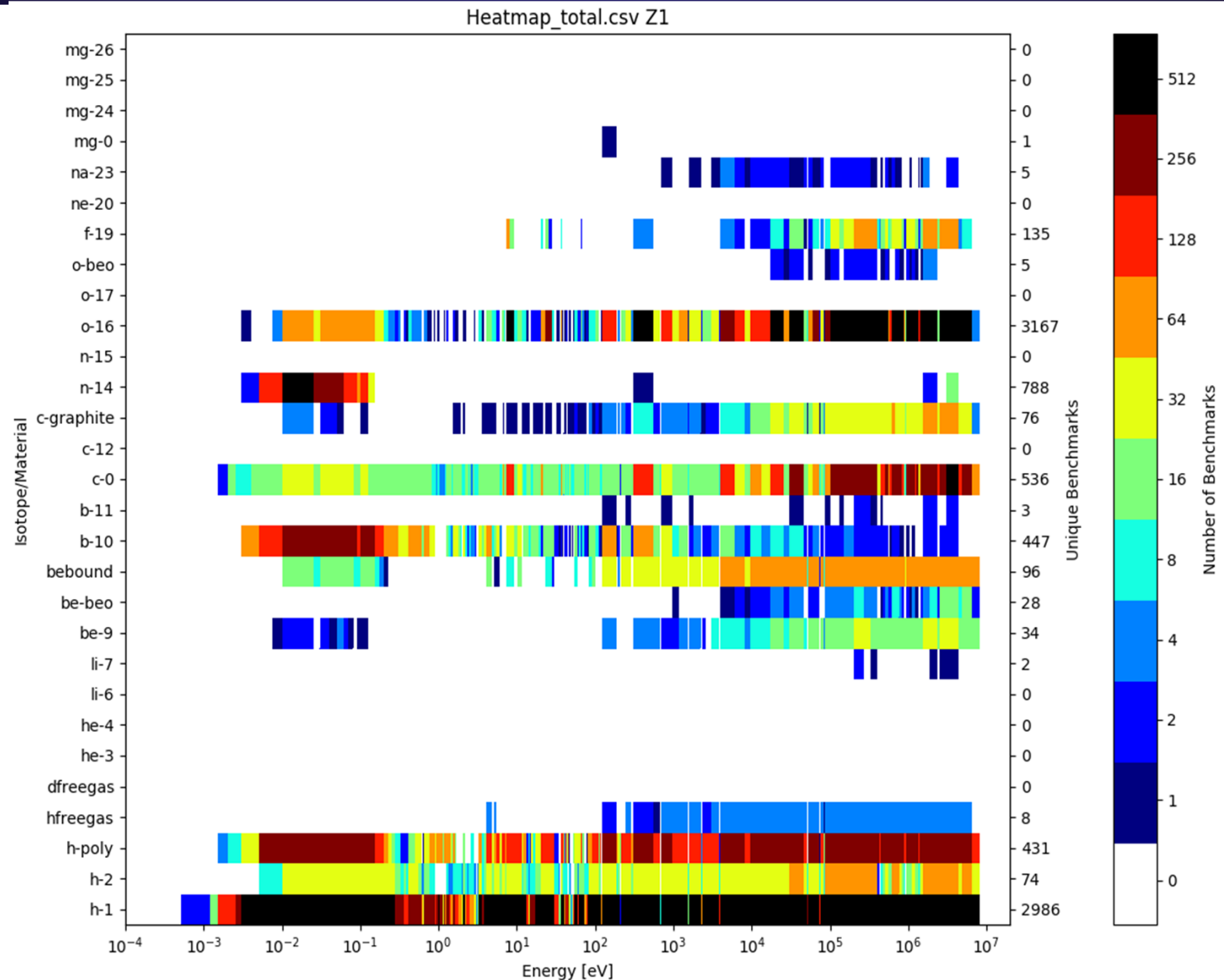
$(C-E)/E$ for U-235 total



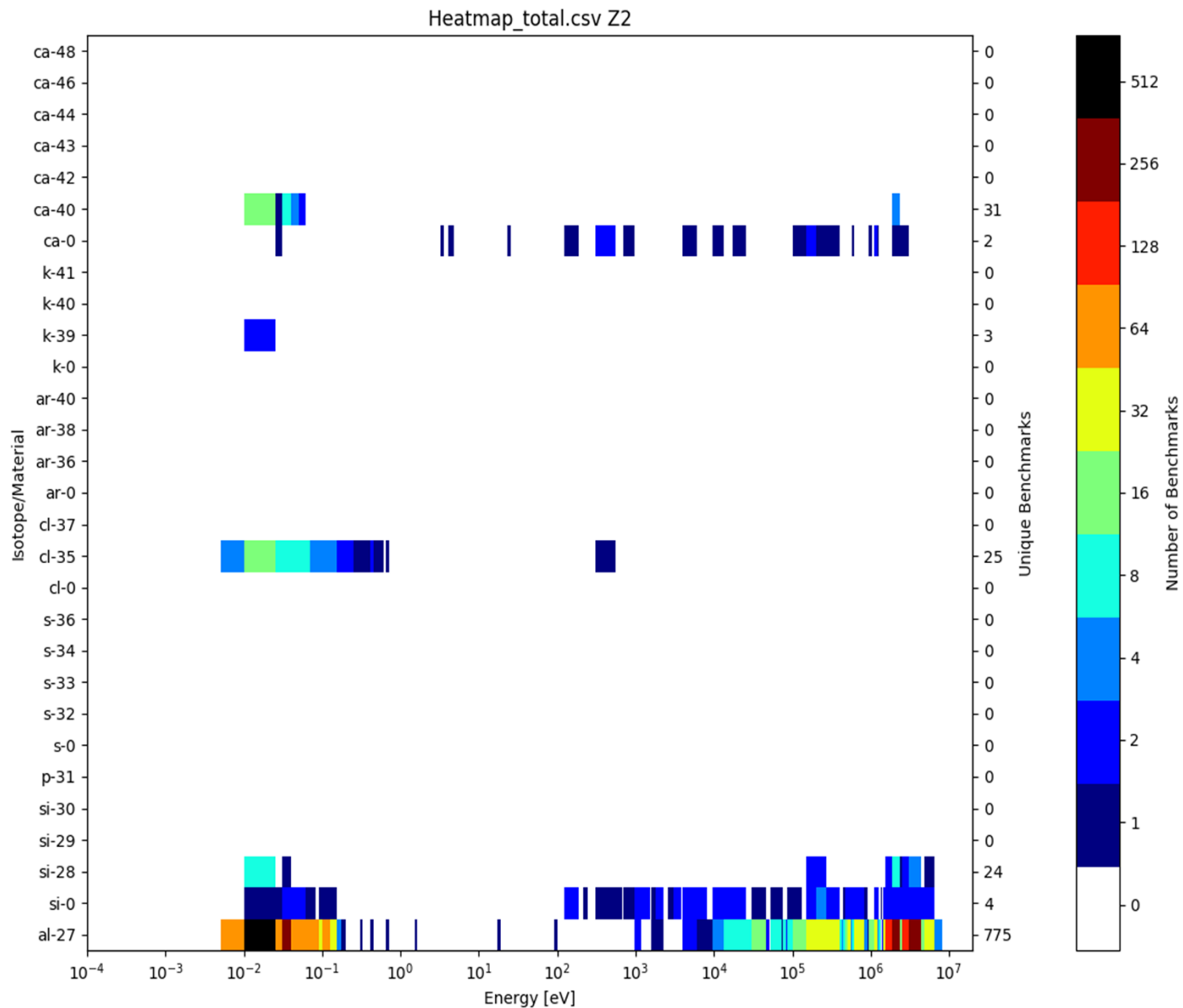
$(C-E)/E$ for U-238 total



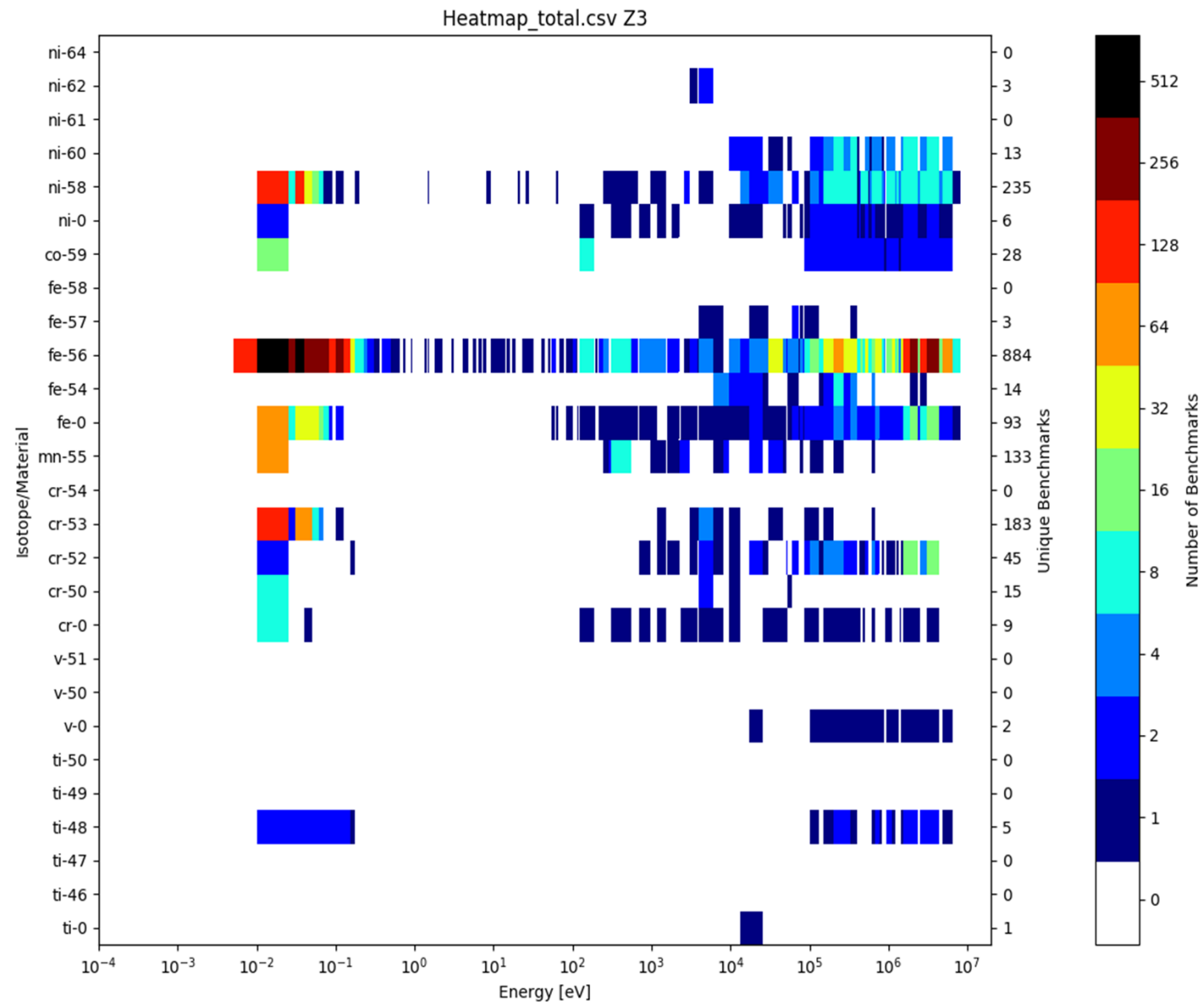
Heatmap – 10^{-3} , Total cross section, (H-Mg)



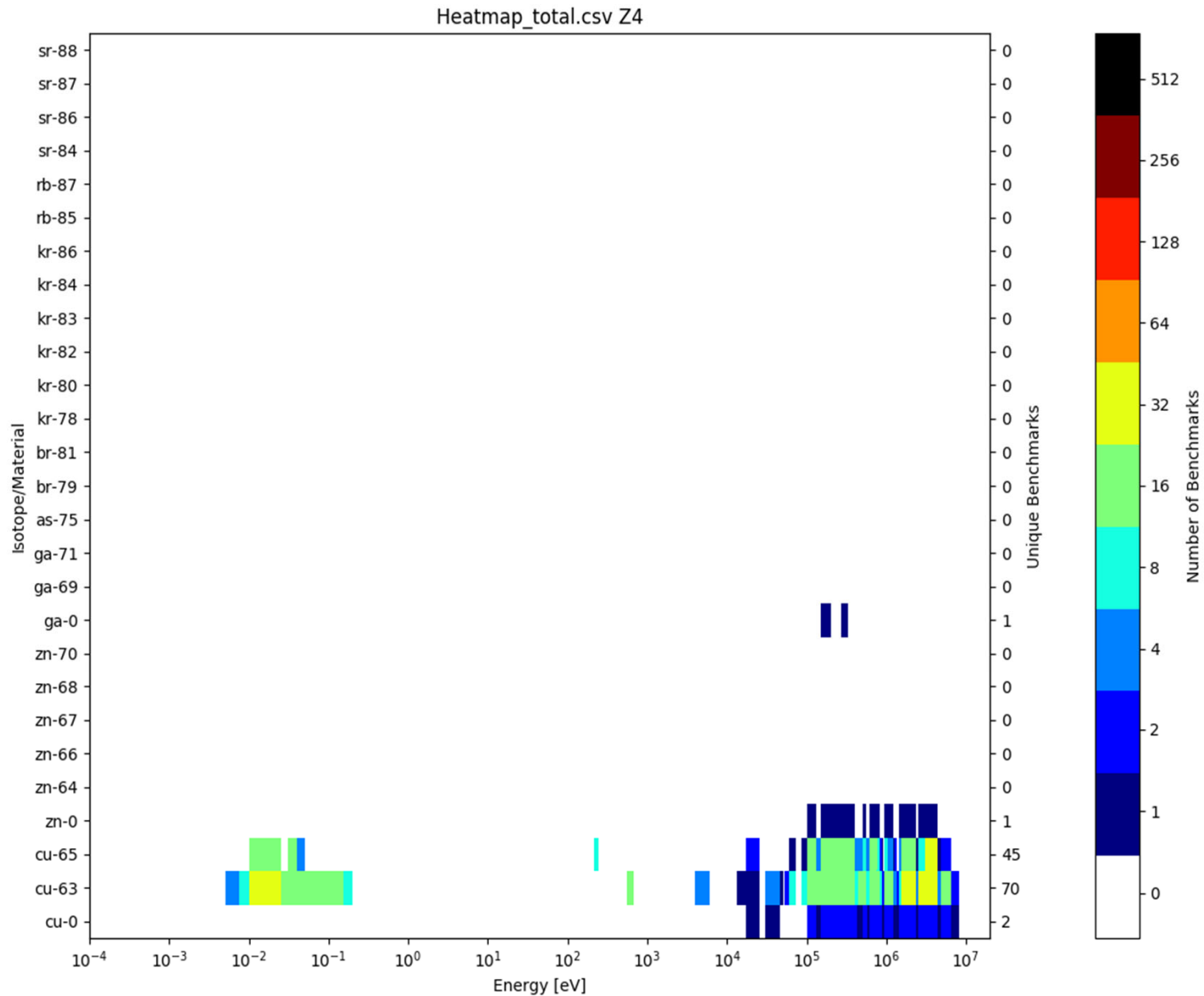
Heatmap – 10^{-3} , Total cross section, (Al-Ca)



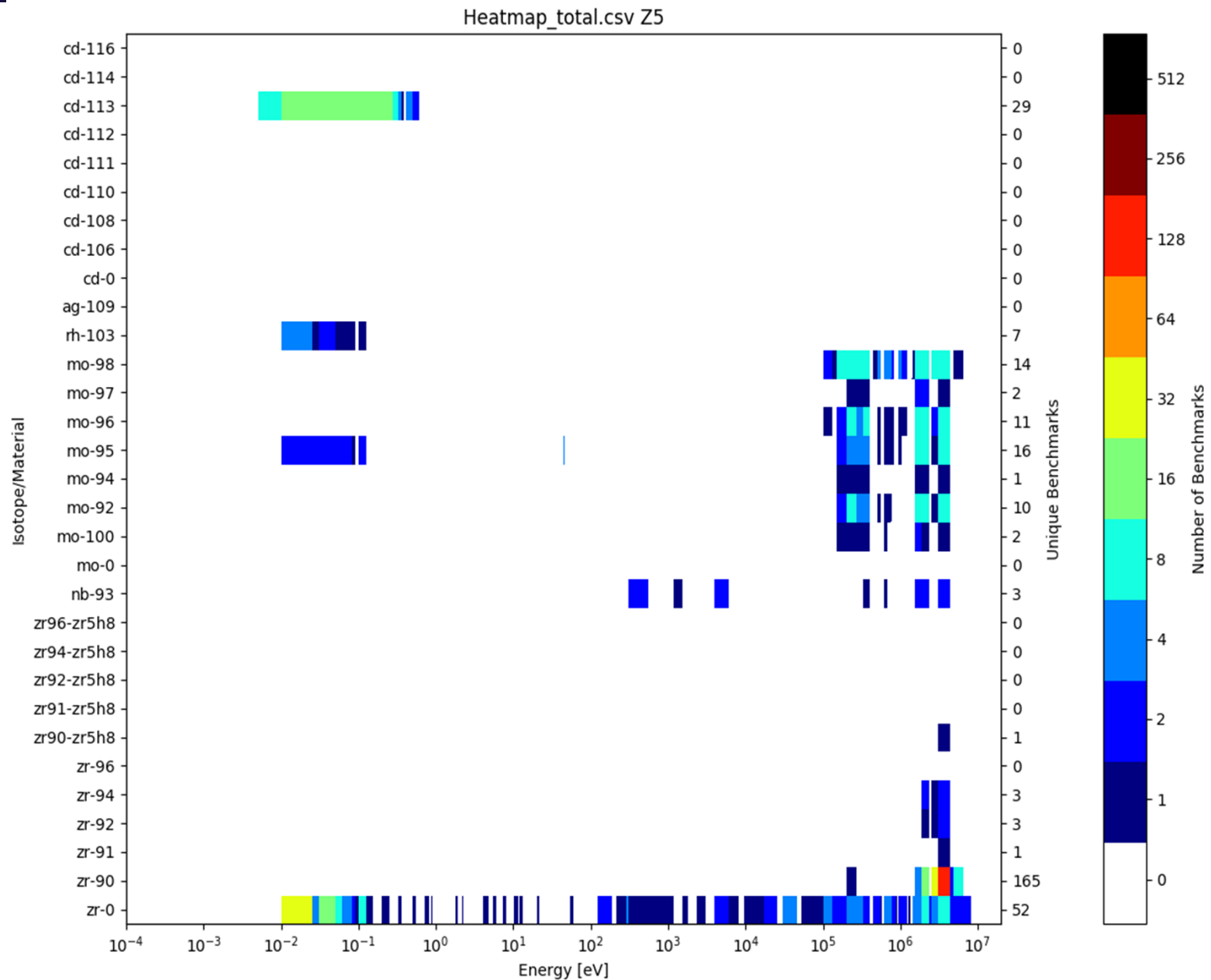
Heatmap – 10^{-3} , Total cross section, (Ti-Ni)



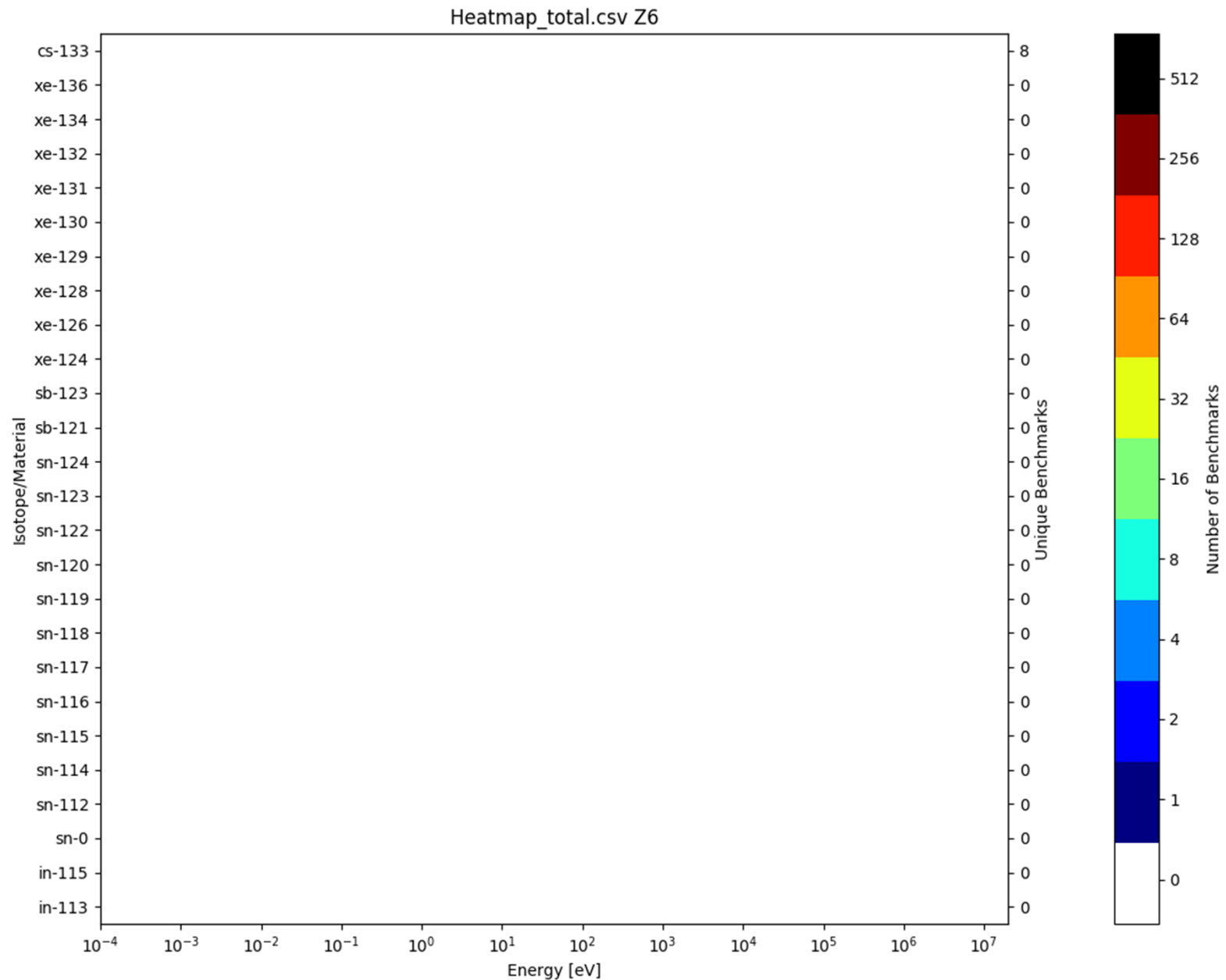
Heatmap – 10^{-3} , Total cross section, (Cu-Sr)



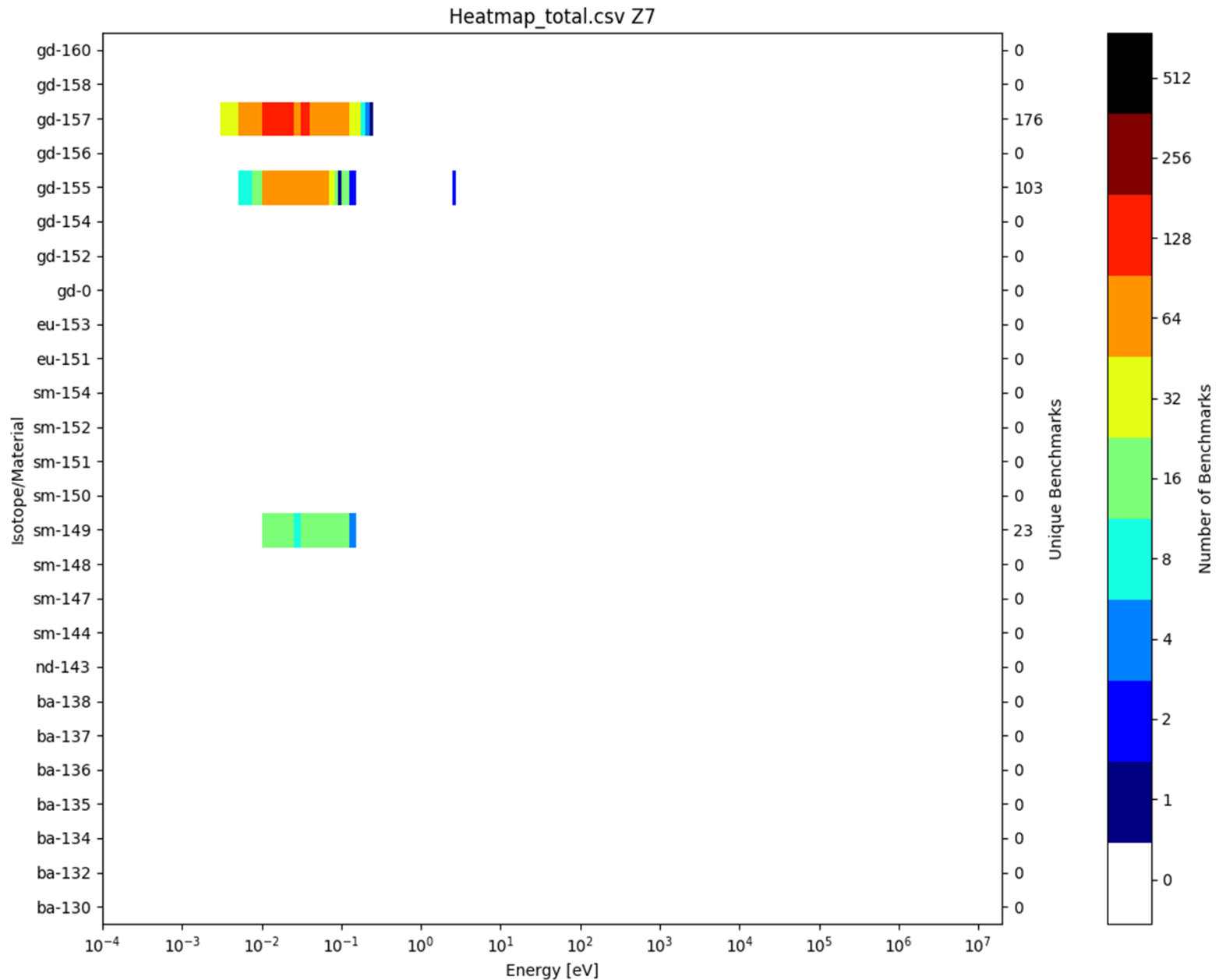
Heatmap – 10^{-3} , Total cross section, (Zr-Cd)



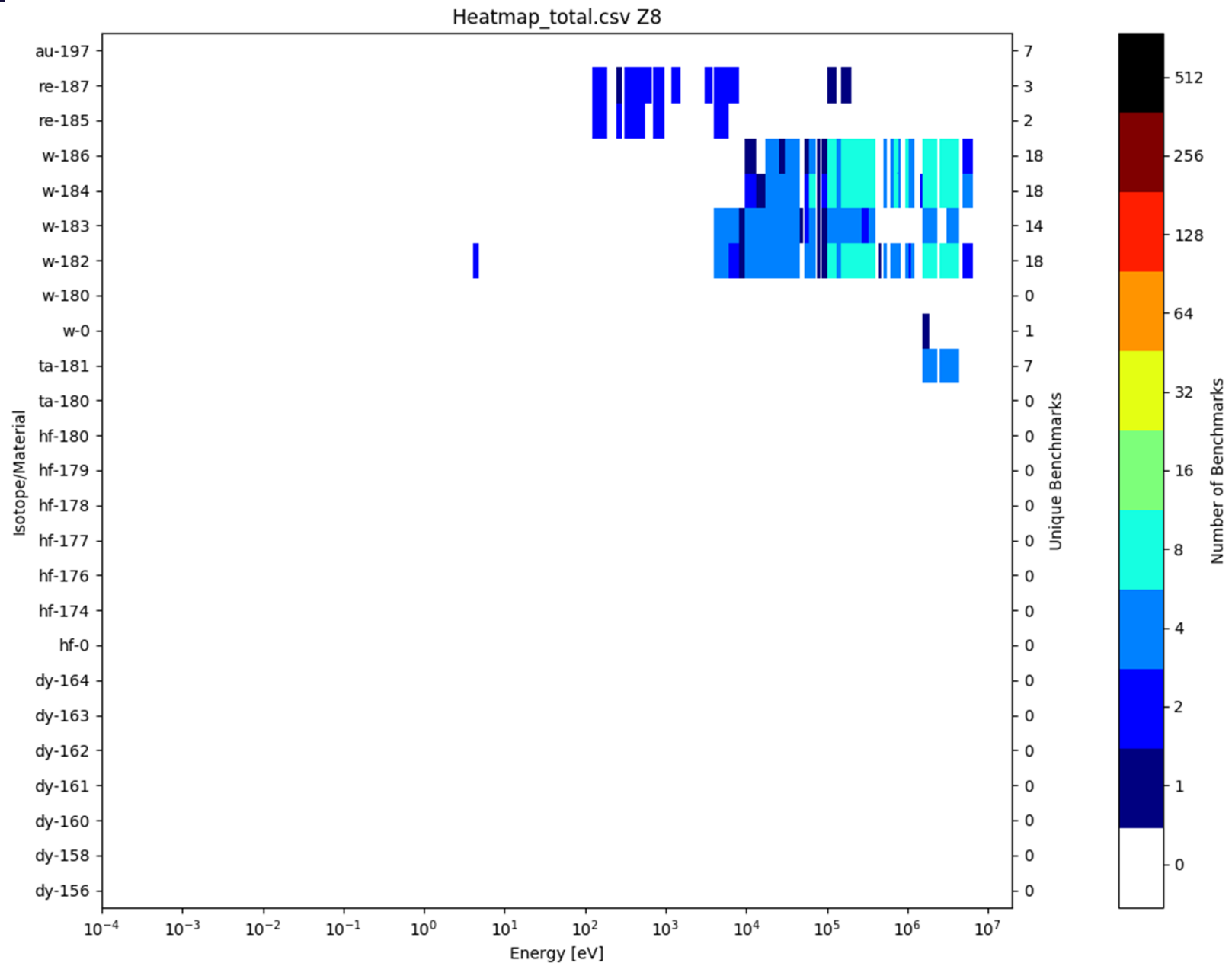
Heatmap – 10^{-3} , Total cross section, (In-Cs)



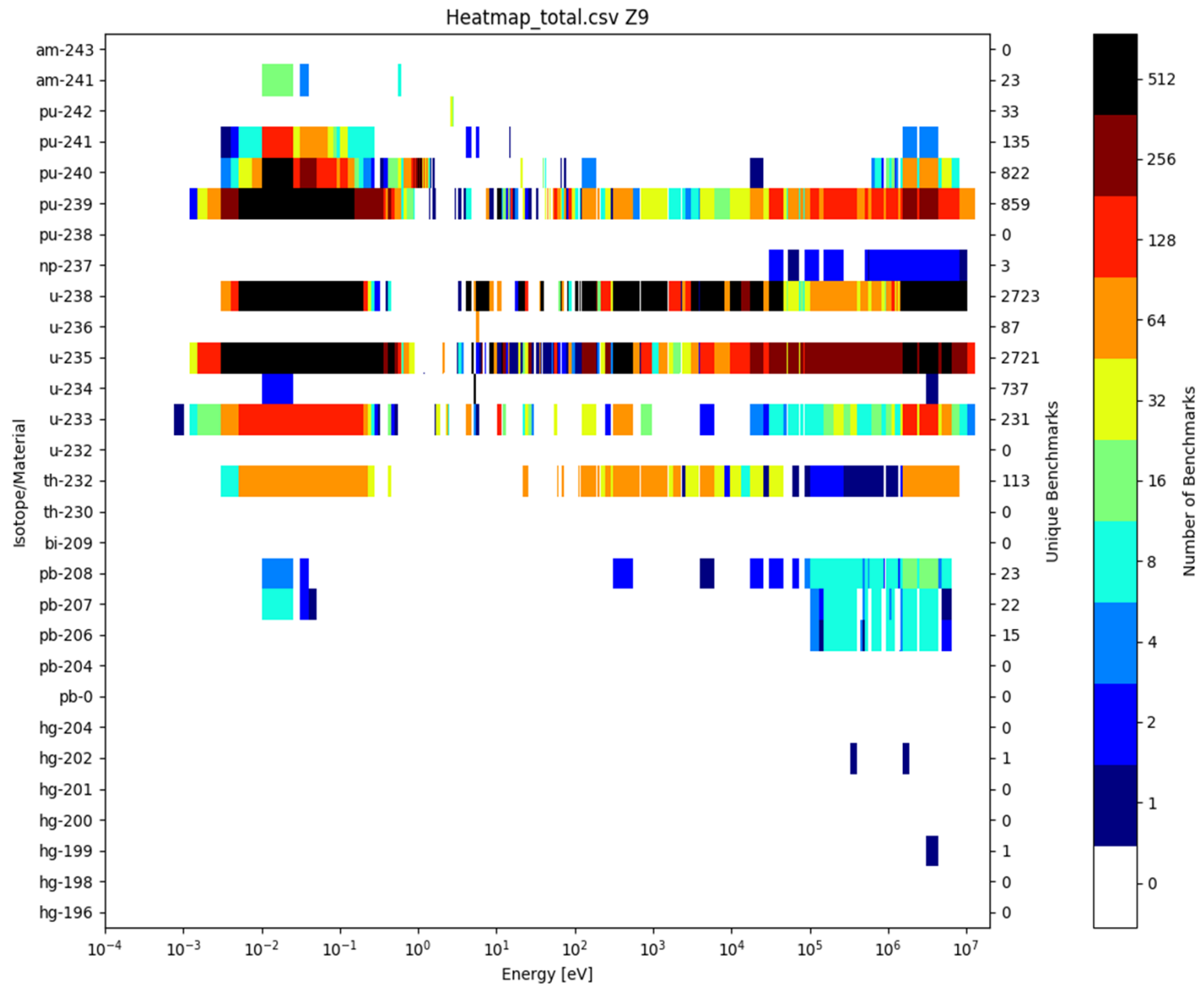
Heatmap – 10^{-3} , Total cross section, (Ba-Gd)



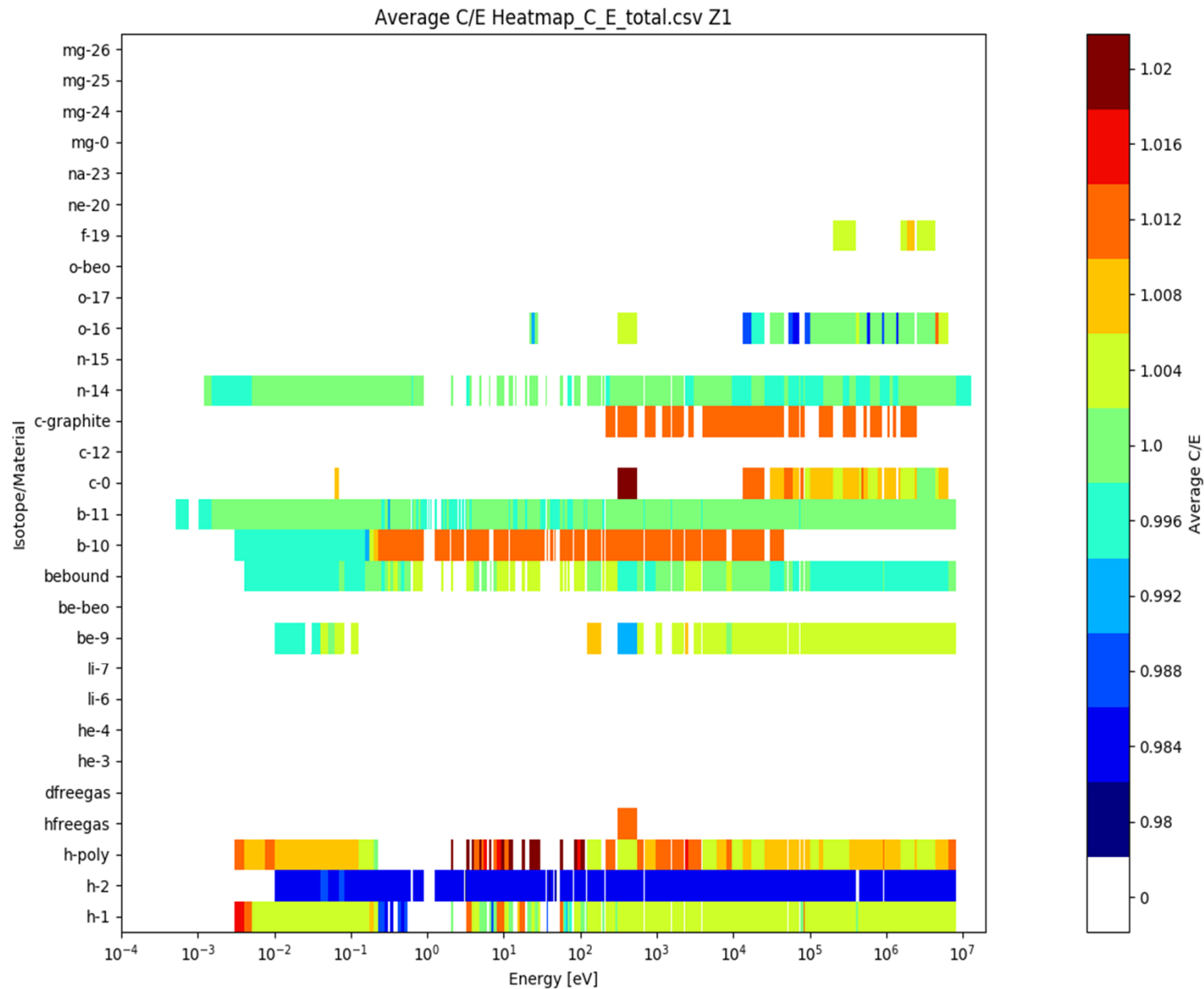
Heatmap – 10^{-3} , Total cross section, (Dy-Au)



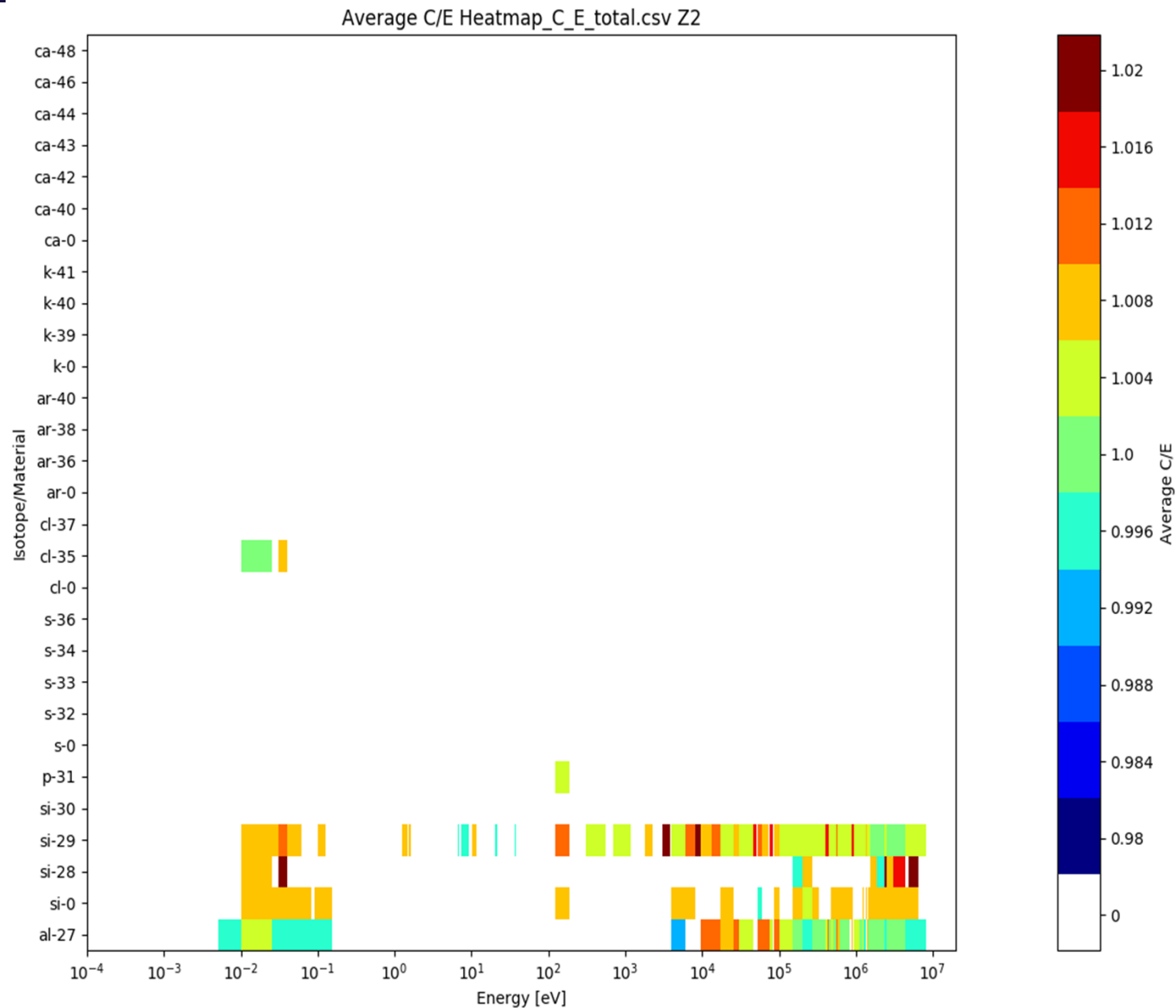
Heatmap – 10^{-3} , Total cross section, (Hg-Am)



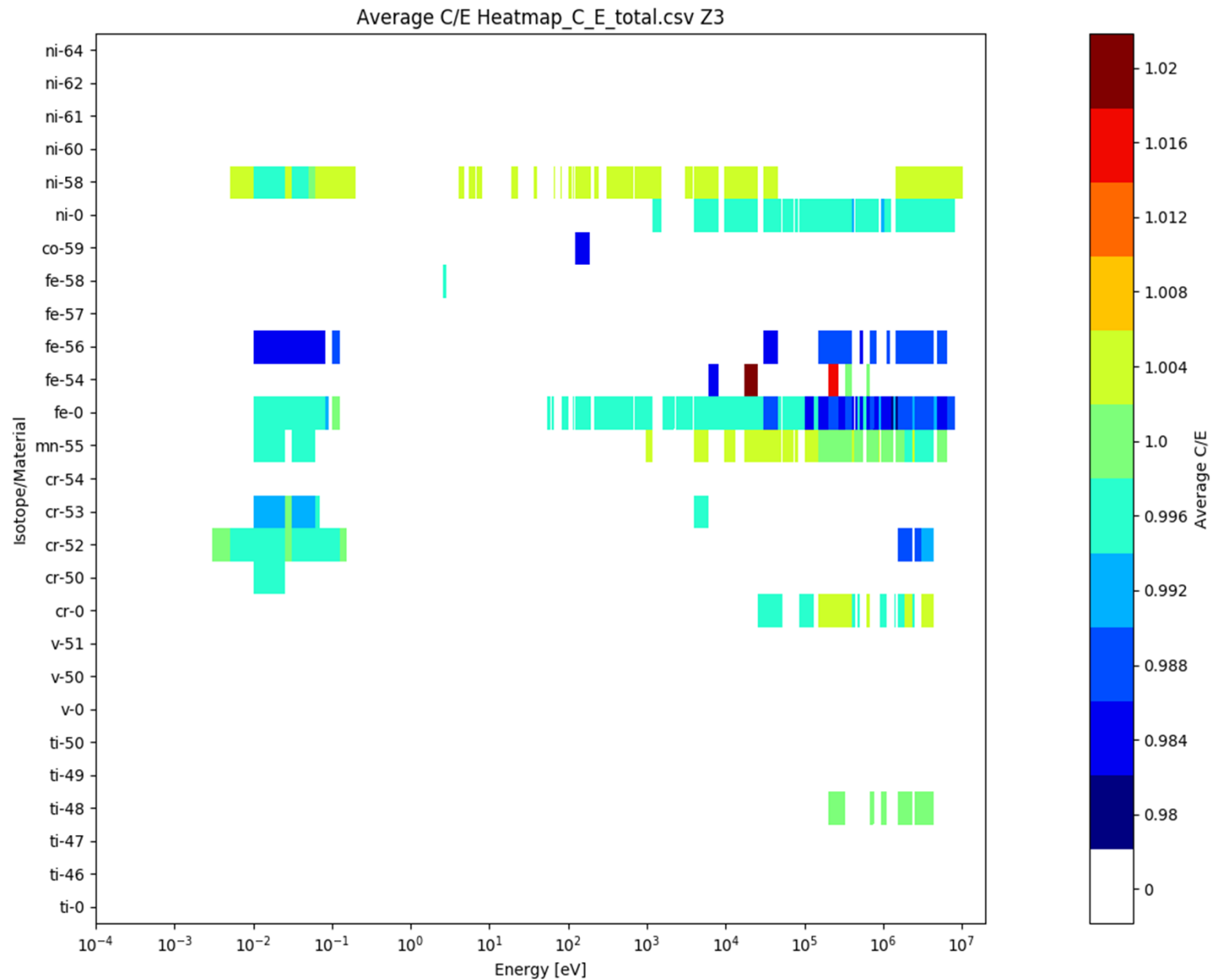
Heatmap – 10^{-3} , Total cross section, (H-Mg)



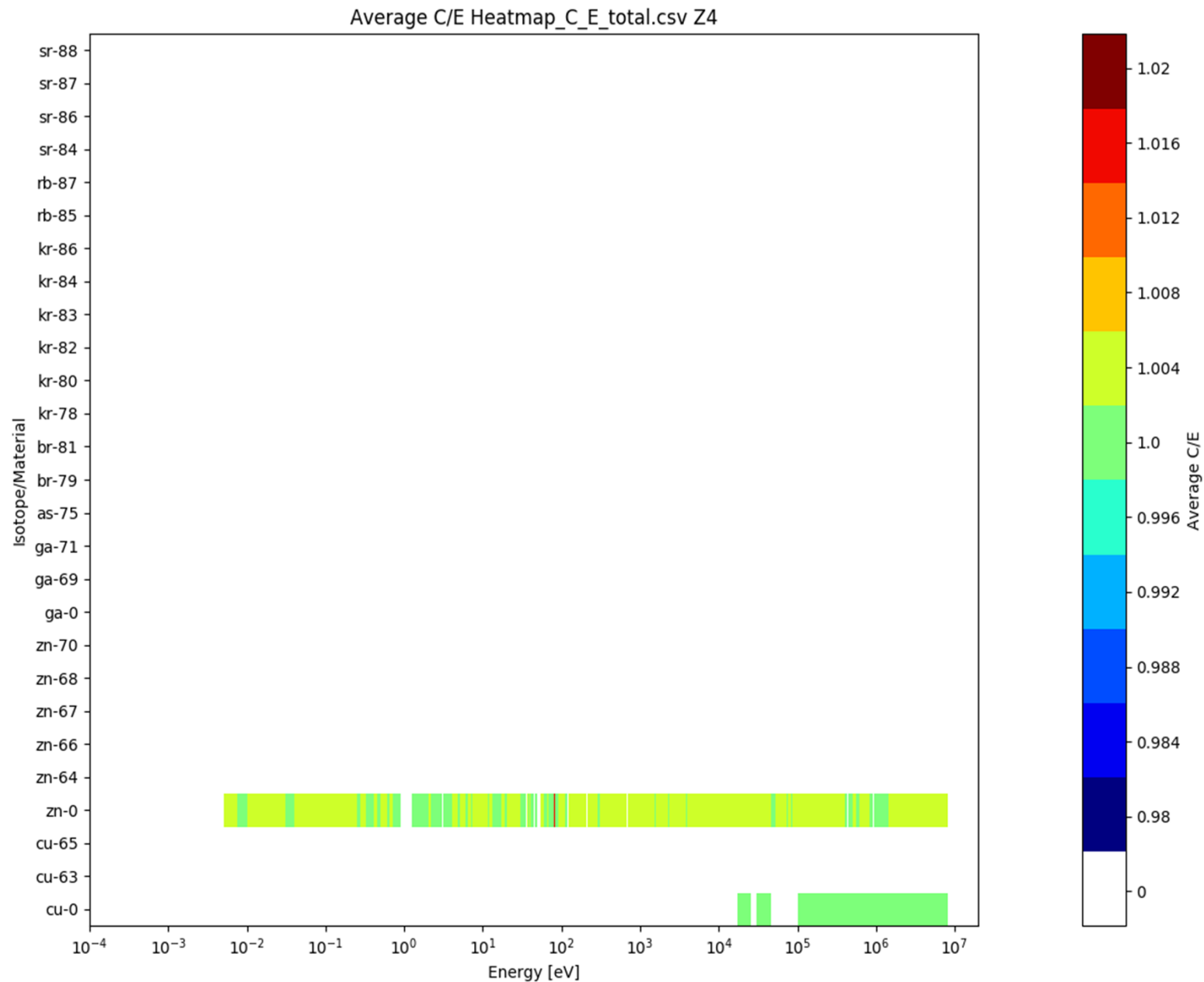
Heatmap – 10^{-3} , Total cross section, (Al-Ca)



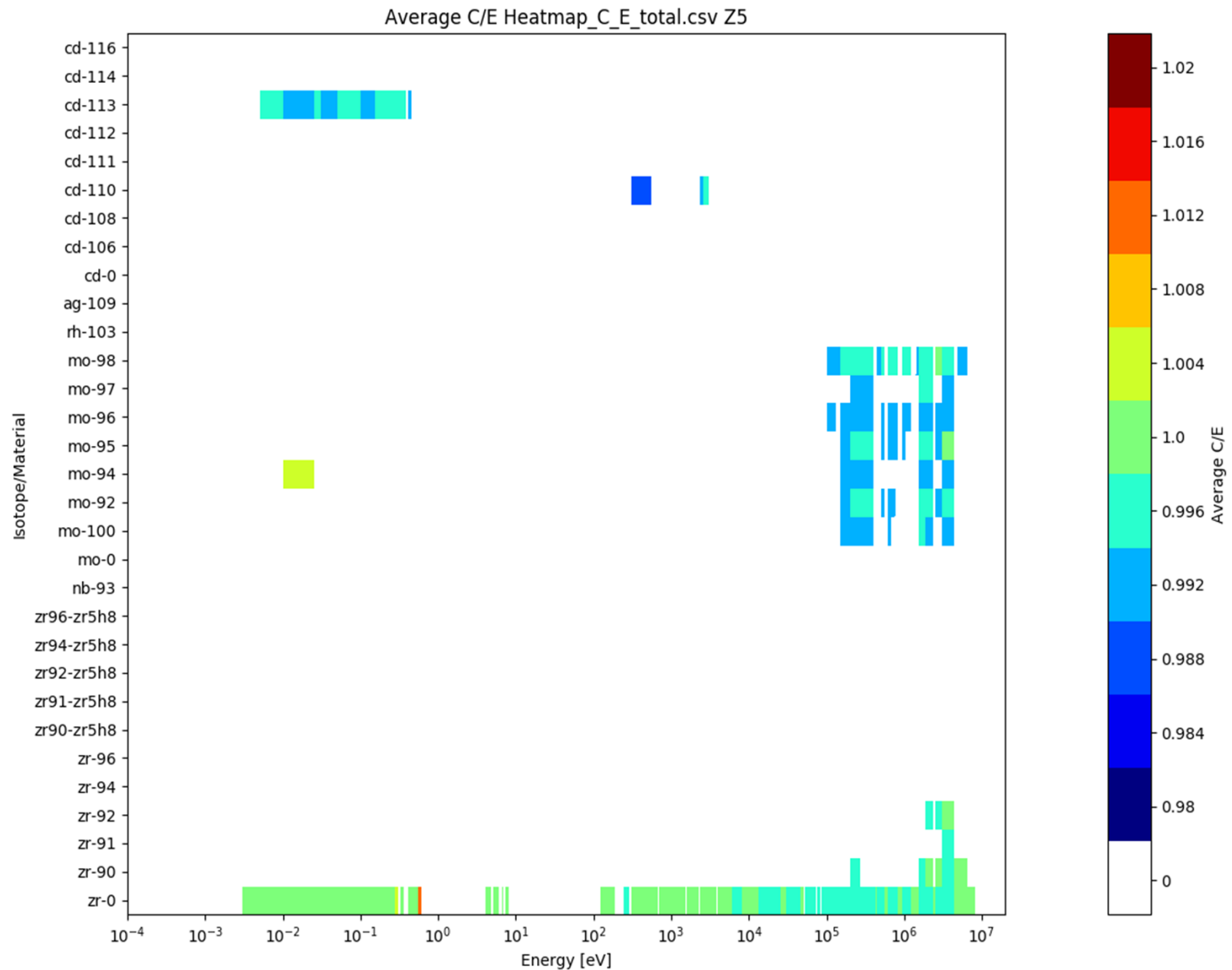
Heatmap – 10^{-3} , Total cross section, (Ti-Ni)



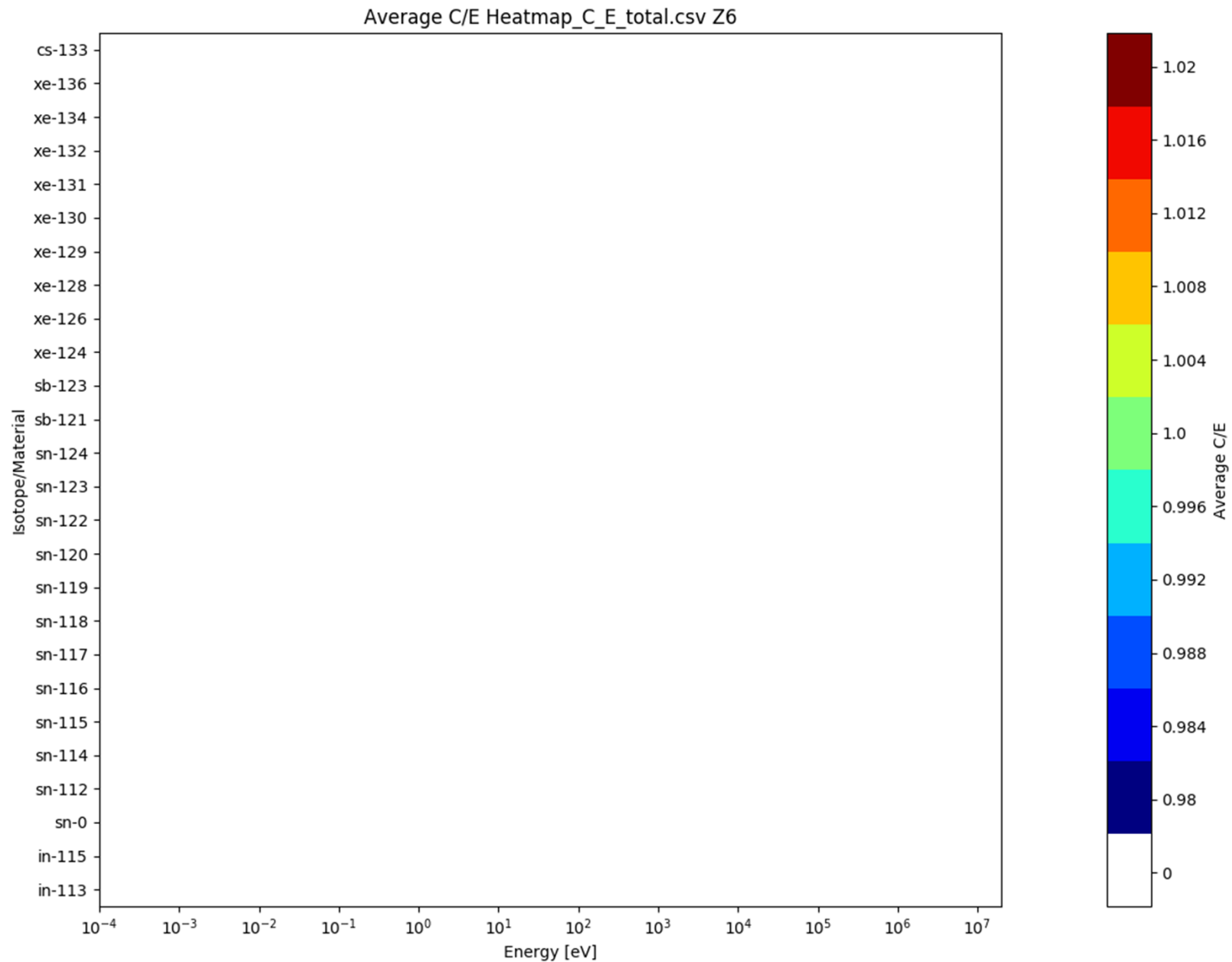
Heatmap – 10^{-3} , Total cross section, (Cu-Sr)



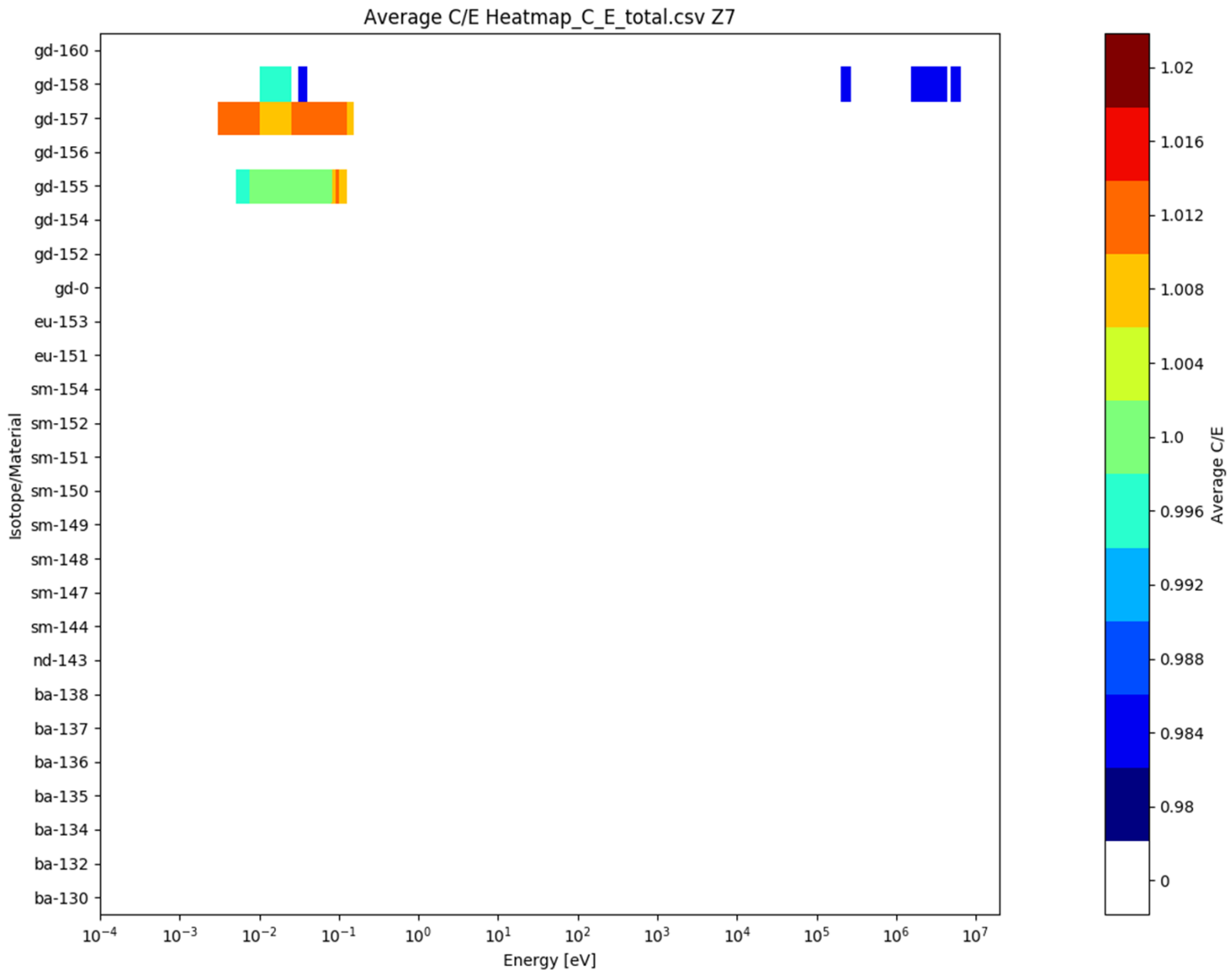
Heatmap – 10^{-3} , Total cross section, (Zr-Cd)



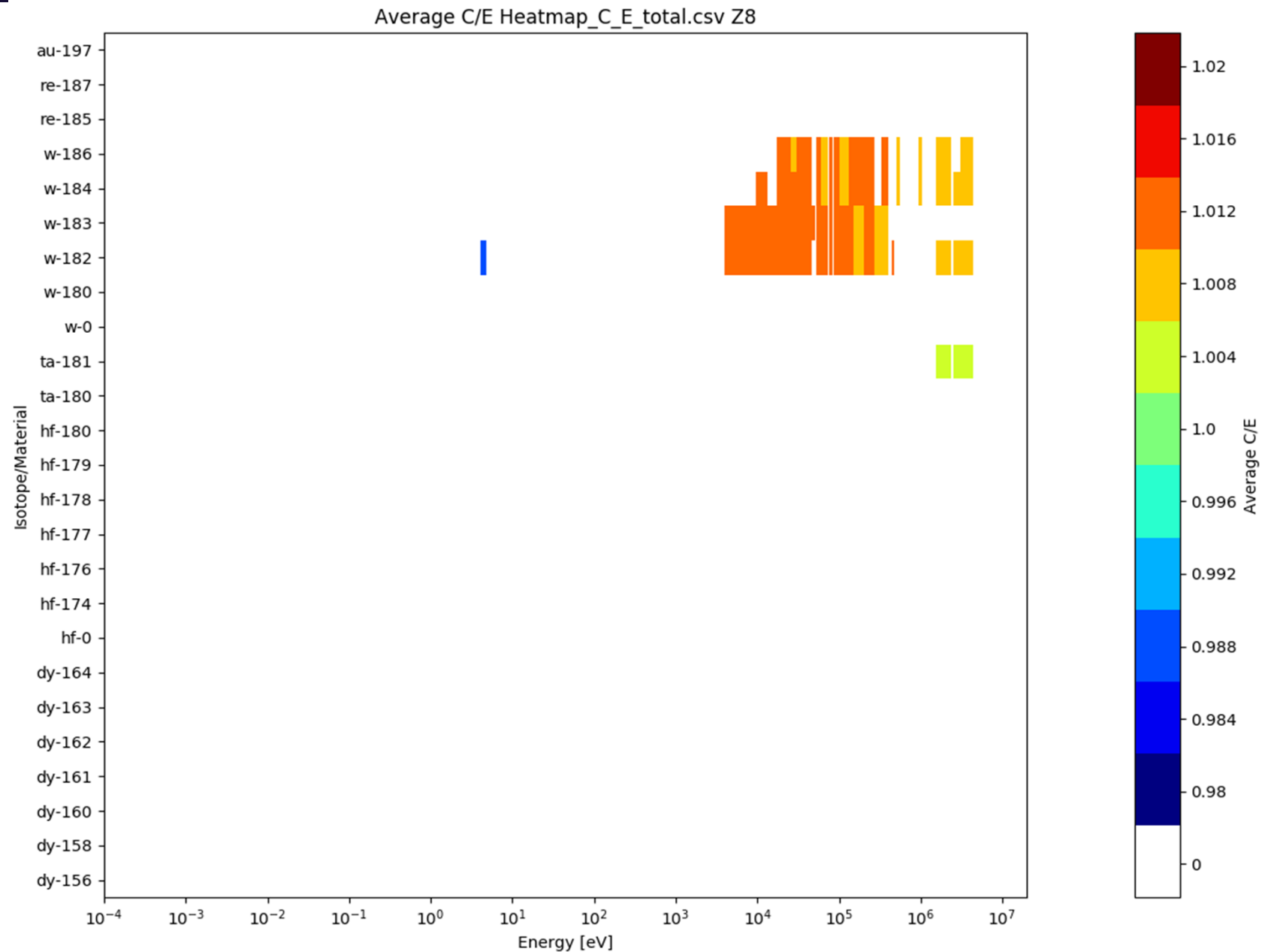
Heatmap – 10^{-3} , Total cross section, (In-Cs)



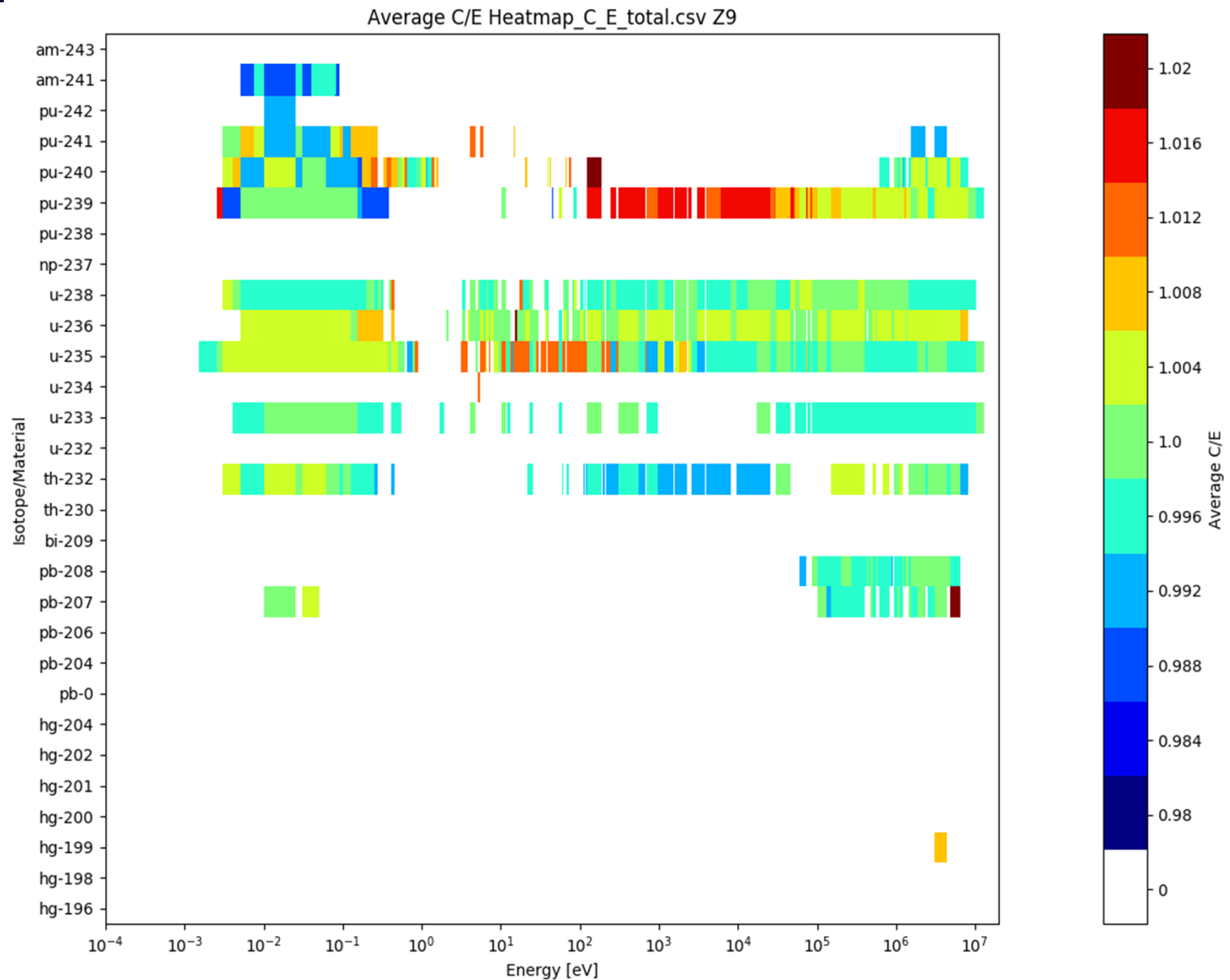
Heatmap – 10^{-3} , Total cross section, (Ba-Gd)



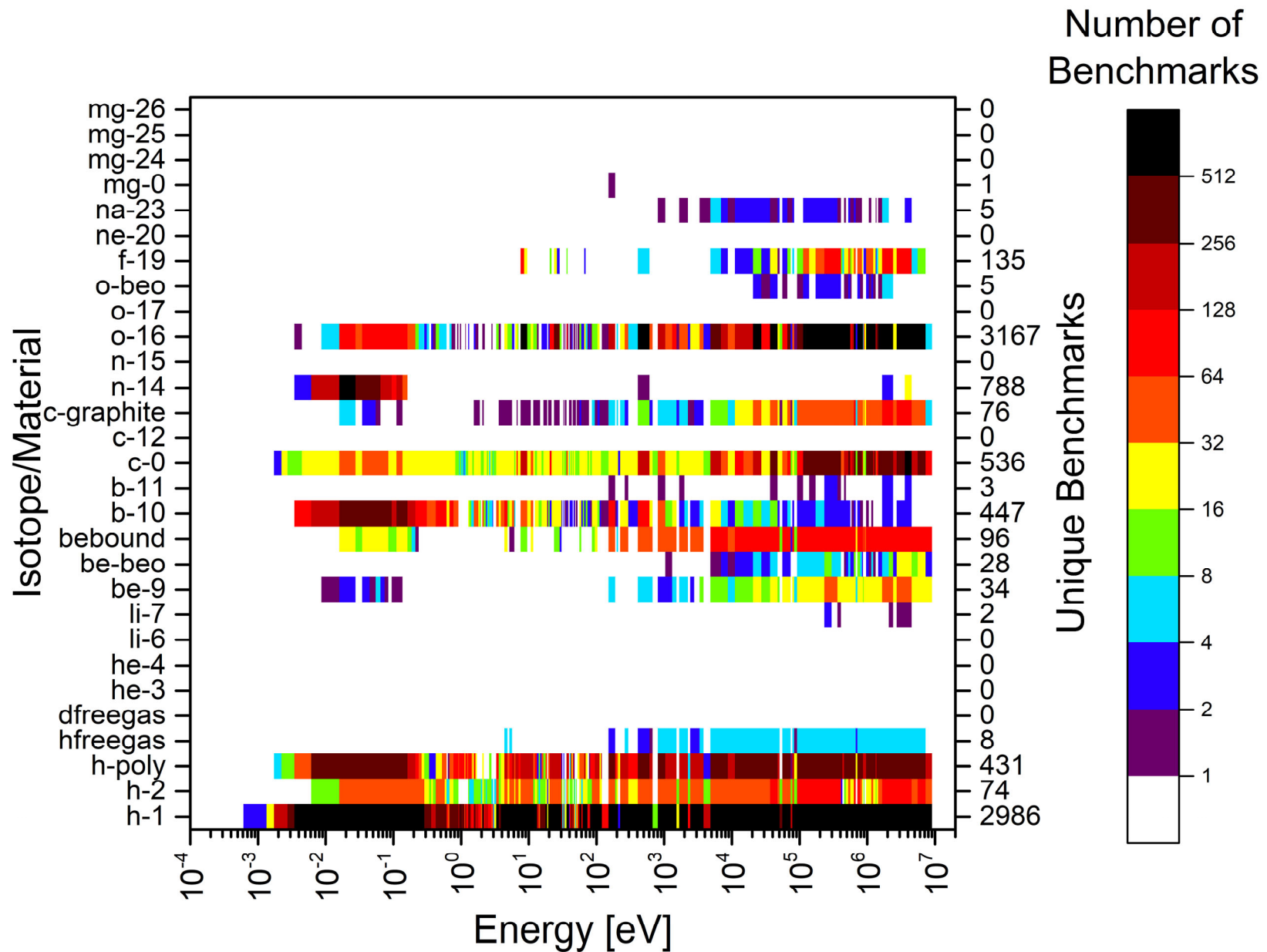
Heatmap – 10^{-3} , Total cross section, (Dy-Au)



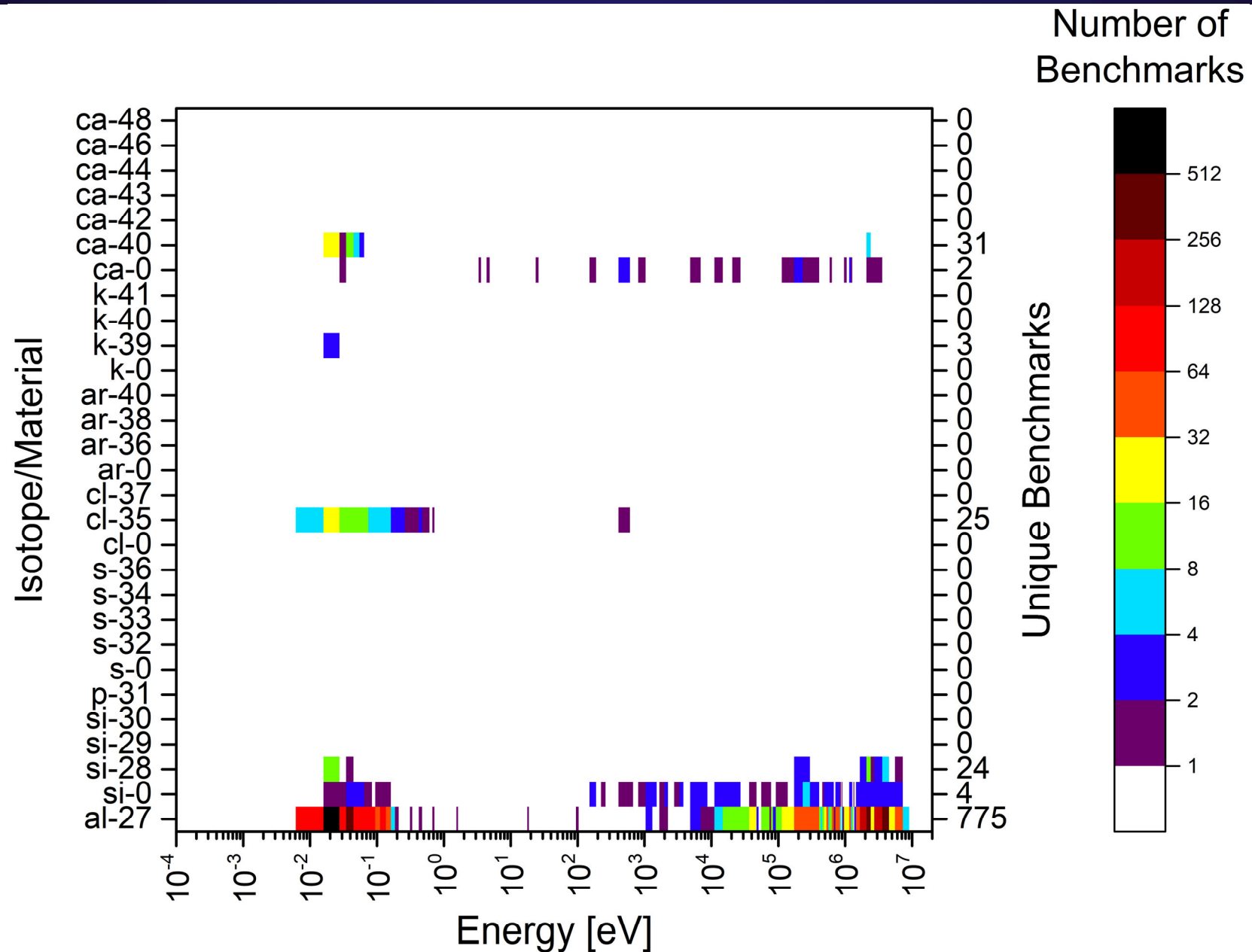
Heatmap – 10^{-3} , Total cross section, (Hg-Am)



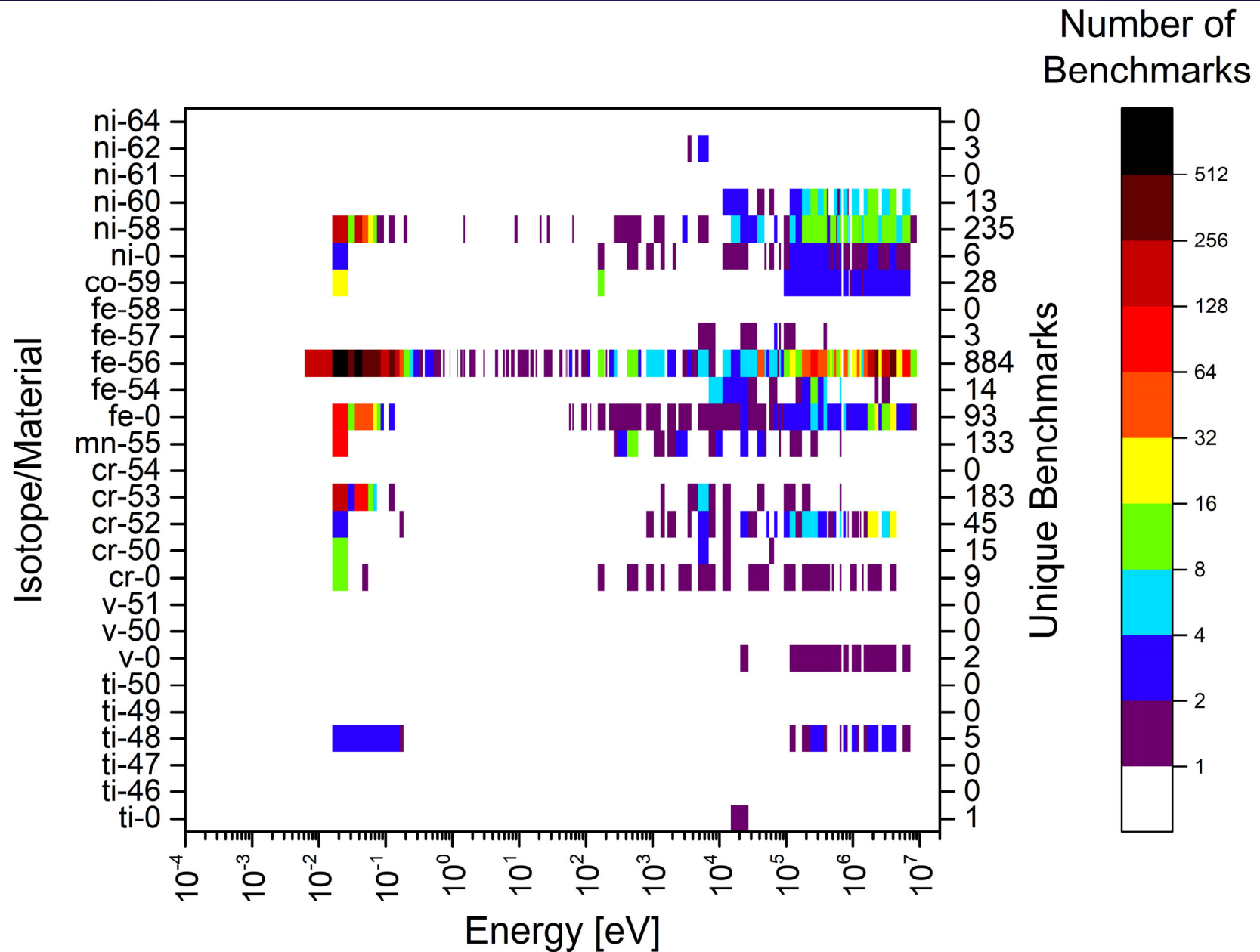
Heatmap – 10^{-3} , Total cross section, Z1 (H-Mg)



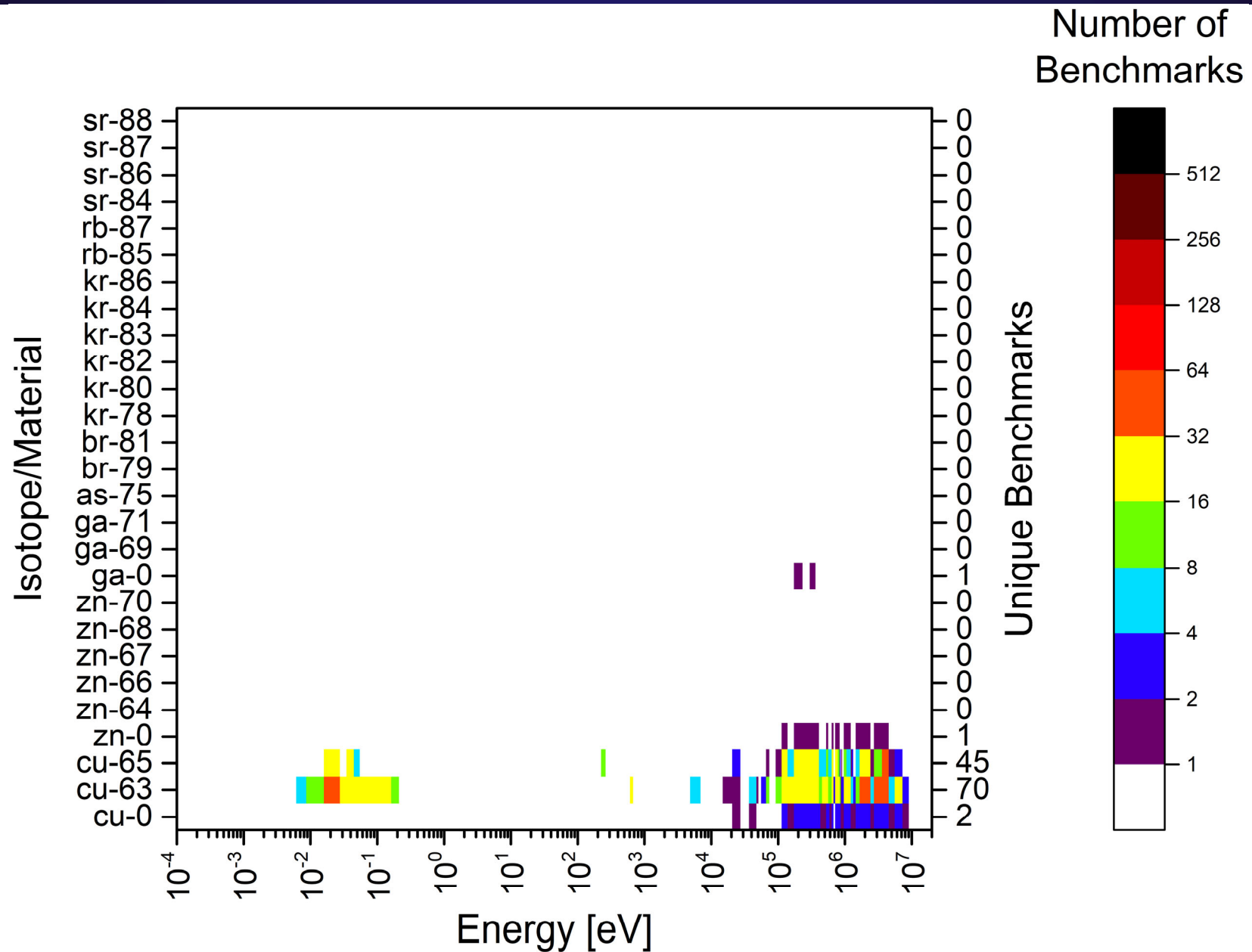
Heatmap – 10^{-3} , Total cross section, Z2 (Al-Ca)



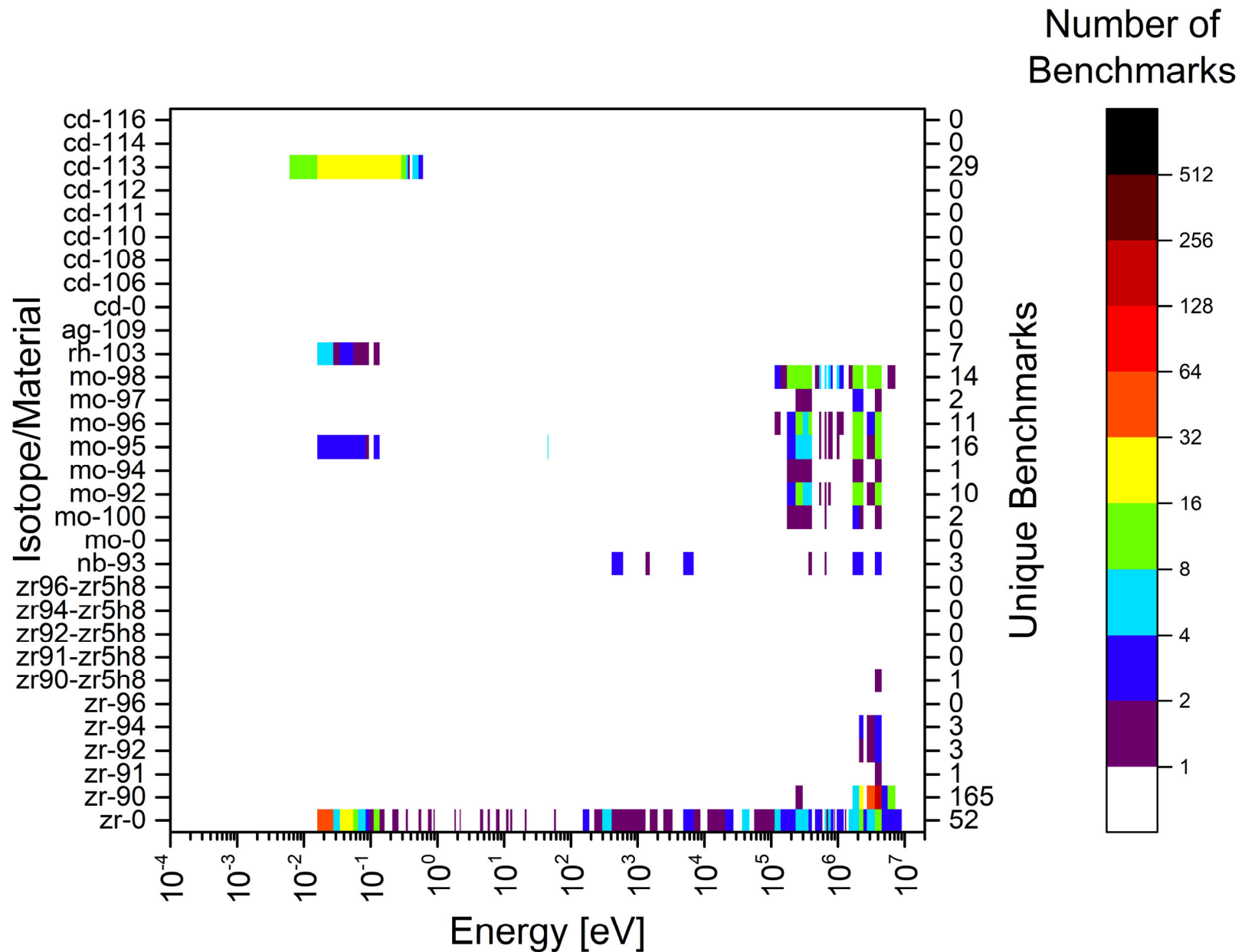
Heatmap – 10^{-3} , Total cross section, Z3 (Ti-Ni)



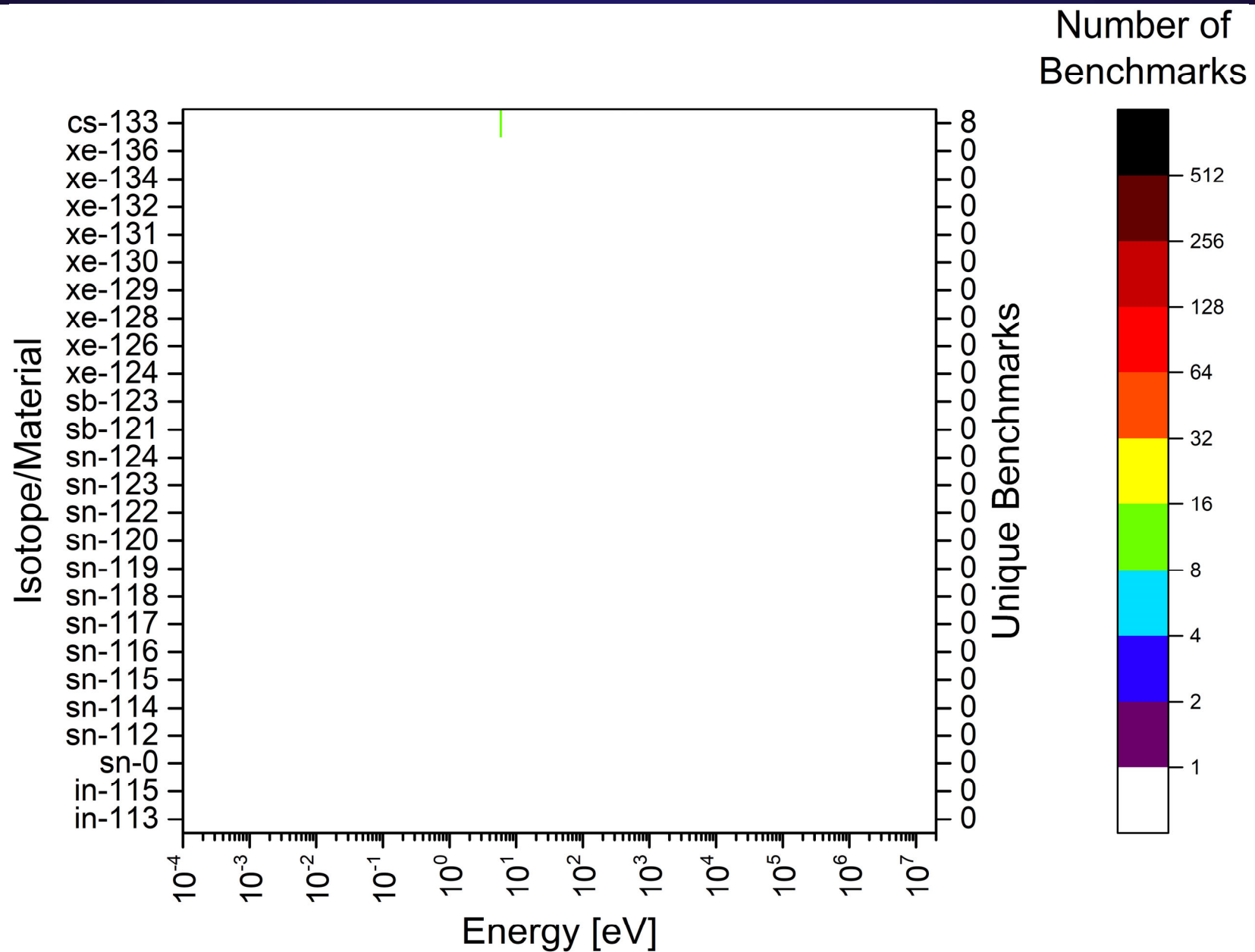
Heatmap – 10^{-3} , Total cross section, Z4 (Cu-Sr)



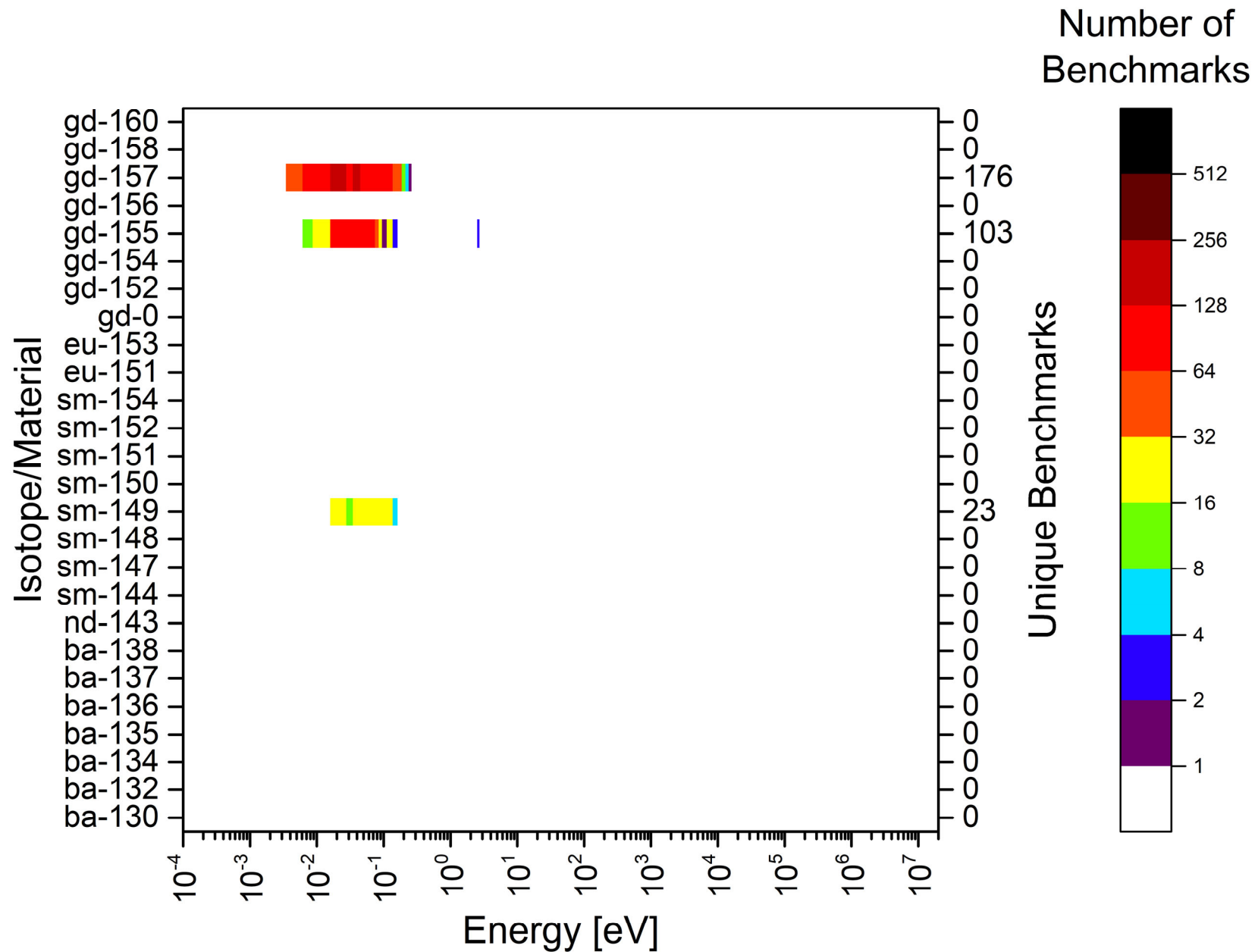
Heatmap – 10^{-3} , Total cross section, Z5 (Zr-Cd)



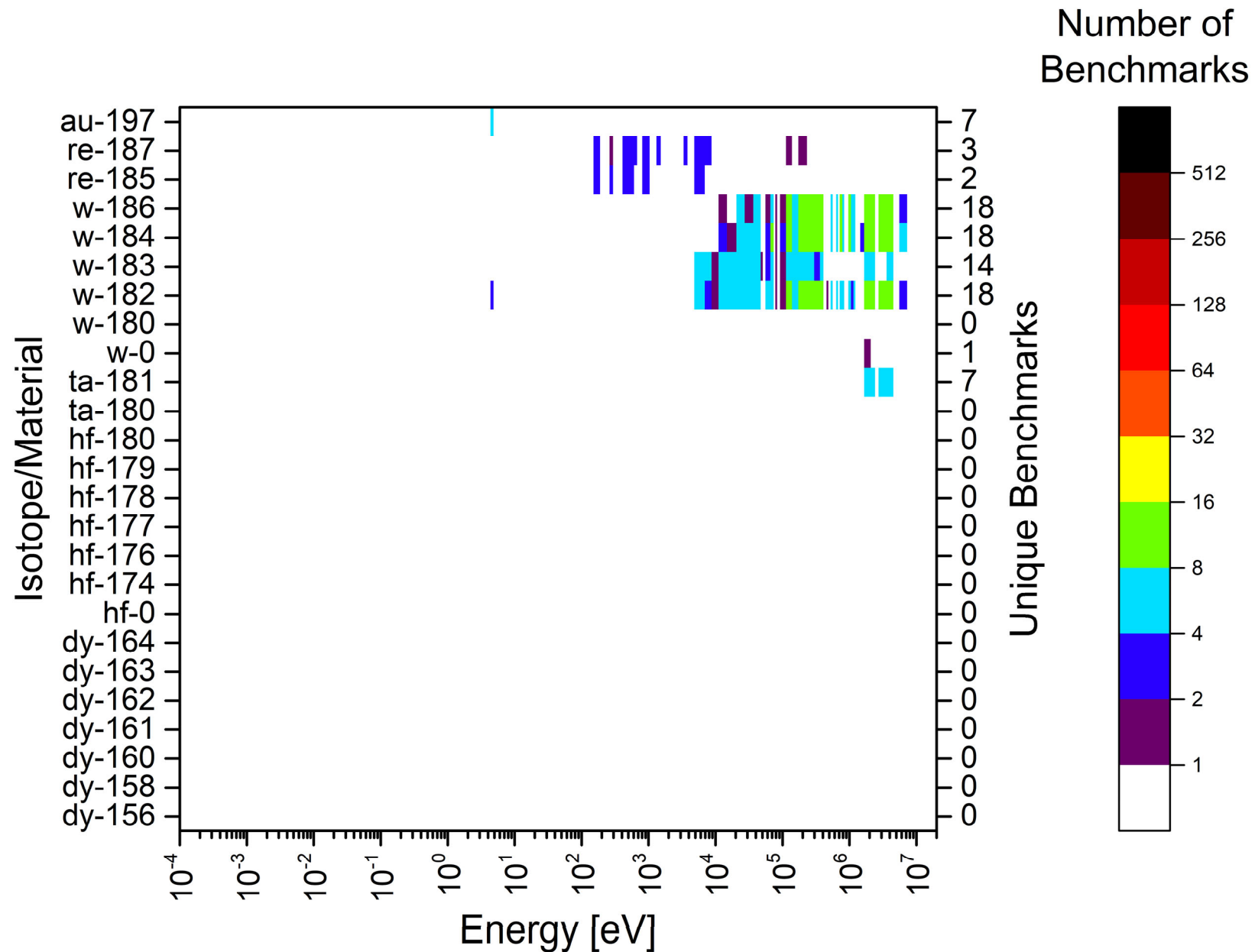
Heatmap – 10^{-3} , Total cross section, Z6 (In-Cs)



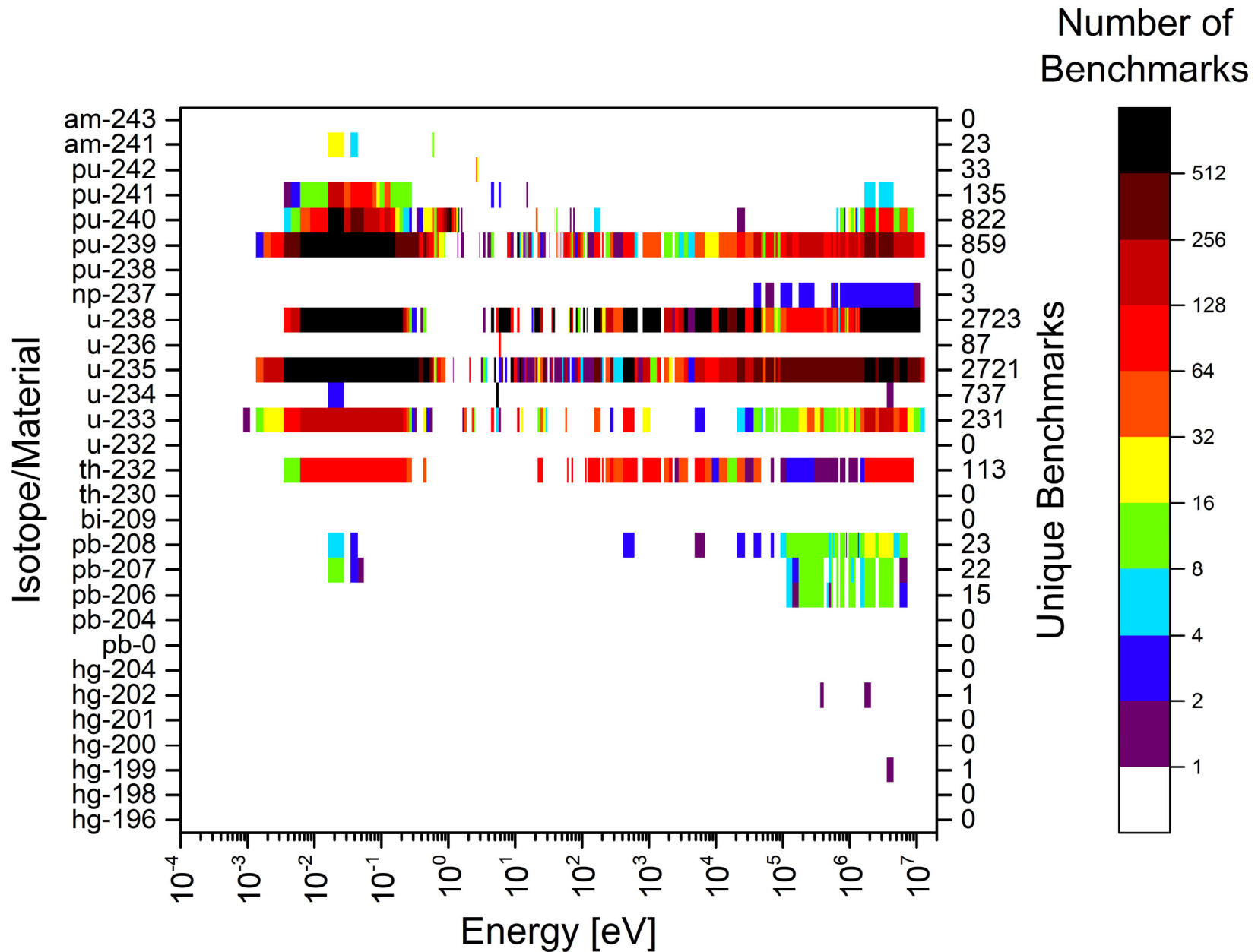
Heatmap – 10^{-3} , Total cross section, Z7 (Ba-Gd)



Heatmap – 10^{-3} , Total cross section, Z8 (Dy-Au)



Heatmap – 10^{-3} , Total cross section, Z9 (Hg-Am)



S.C. van der Marck – Benchmarking with MCNP6 paper

- He looked at many, many benchmarks, sorted them by materials
- **Simulated them using ENDF/B-VII.1, JENDL-4.0, and JEFF-3.1.1 libraries**
 - Enormous number of results, and enormous amount of simulation time (CPU years)
- **Three categories of benchmarks:**
 - Criticality
 - Shielding
 - 14 MeV neutrons surrounded by various materials
 - Delayed neutron fraction - Rossi- α and β_{eff}
- **Criticality benchmarks**
 - LEU (<10% wt% ^{235}U), IEU, or HEU (> 60%)
 - Metal, compounds, and solutions
 - Thermal, Intermediate, Fast, Mixed Energy Spectrum
 - Thermal defined as >50% of fissions occur under 0.625 eV,
 - Fast defined as >50% of fissions occur above 100 keV,
 - Intermediate defined as >50% of fissions occur between 0.625 eV and 100 keV,
 - “Mixed” energy spectrum is if none of those conditions are met

S.C. van der Marck – Benchmarking with MCNP6 paper

- **One example, benchmarks with Cd**
 - Benchmarks with LEU, in a compound (eg. UO_2), with a thermal spectrum agree very well (lct12 is an outlier)
 - Benchmarks with HEU metal fuel aren't great
 - Benchmarks with HEU in a solution are all over the place – and JEFF-3.1.1 significantly disagrees with ENDF/B-VII.1 or JENDL-4.0

All of these have a thermal spectrum – why do some agree and others don't, and why does JEFF-3.1.1 basically agree with ENDF/JENDL everywhere except hst49?

“Thermal” is not descriptive enough!

TABLE XXXVI: Average values for $C/E - 1$ (in pcm) for benchmarks containing Cd. N is the number of benchmarks in the category.

Category	N	ENDF/B-VII.1	JENDL-4.0	JEFF-3.1.1
leu-comp-therm	19	-155	-127	-171
ieu-comp-therm	2	-293	-308	-569
heu-met-therm	2	-457	-504	-698
heu-sol-therm	29	-270	-167	-745
pu-met-fast	1	631	486	339

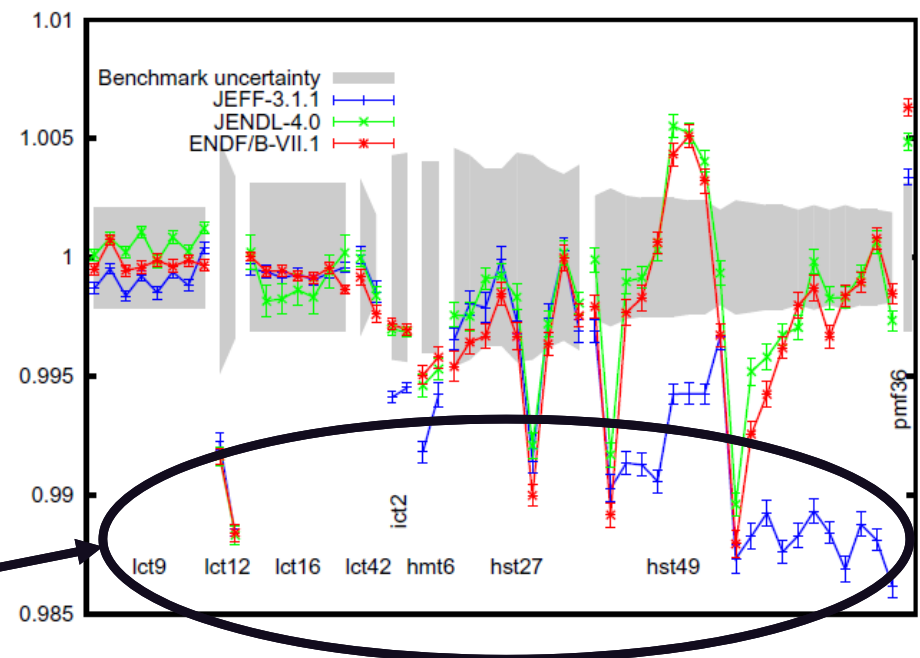


FIG. 34: The results for criticality safety benchmarks containing Cd, C/E .

Separating by Fast/Thermal/Intermediate/Mixed is good, but not sufficient.

S.C. van der Marck – Benchmarking with MCNP6 paper

- **Conclusions:**

- van der Marck makes some suggestions about looking at correcting nuclear data for certain elements (Fe, Gd, etc.)
- He does not make suggestions about what integral benchmarks are missing or would be useful (what gaps there are in benchmarks)
 - This is somewhat application specific – eg. commercial nuclear reactors aren't that concerned about fast and intermediate cross sections.
- He also does not look at benchmarks with different temperatures
 - Important for reactors and for testing thermal scattering libraries