IAEA

Predictive power of TALYS

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Contents

- Introduction
- Global quality of level density and photon strength function
- EXFOR cleanup
- MACS database
- Neutron reactions up to 30 MeV
- Summary

Short-lived nuclides?

Number of target nuclides:
Stable: 287
τ > 1 year + stable: 407
τ > 1 day + stable: 675
τ > 1 hour + stable: 995
τ > 1 sec + stable: 2854

Nuclides with EXFOR cross sections:
(n,tot): 347
(n,el): 223
(n,γ): 402
(n,f): 32
(n,n'_1): 176
(n,2n): 198
(n,p): 212
(n,α): 169

Exp. nuclear structure:
Discrete levels: ~1200
Masses: 2550 (3558)

Nuclides in nuclear data libraries:
ENDF/B-VIII.1: 495
JENDL-5.0: 667
JEFF-4.0: 547
TENDL-2023: 2854

Material	Experimental data	Nuclear models	Evaluation/Validation
(1) The Big Three: ^{235,238}U, ^{239}Pu	High-quality measurements (< 2 % for important channels), directly (cor)related with neutron standards More than 10-20 exp. data sets in same energy range	Models overruled by experimental data for important channels: complete normalization of model results	Need for reliable experiment-based covariance data Direct feedback from integral measurements: criticality, reactor systems, inventory, etc.
(2) Important coolants and structural materials: H, C, O, Fe	Many experimental data sets for many channels uncertainty < 10% (dosimetry reactions < 3 %)	Precise nuclear model calculations with many parameters to interpolate between measurements	Sometimes differential data overruled by data with better integral performance
(3) Other coolants and structural materials: N, Na, Al, Si, Ti, V, Cr, Mn, Ni, Cu, Zr, Mo, W, Pb, Bi,...		Parameter adjustment for well-measured channels	
(4) Other important actinides: ^{232}Th, ^{233}U, $^{240-242}$Pu	Many experimental data sets for only the most important channels	Models used for almost all secondary distributions (angles, spectra, photons, etc.)	Isolated benchmarks available for transport or activation analyses
(5) Important fission products: ^{99}Tc, ^{103}Rh, ^{129}I,....			
(6) Breeding materials and reflectors: Li, Be,...		Model calculations with a few parameters adjusted to the few exp. data sets	
(7) Absorbers: Gd, Hf,...			
(8) Minor actinides: ^{241,242m,243}Am, ^{237}Np,....	Experimental data only available for (low energy) total, elastic, capture (resonance parameters) and a few other channels		Global covariance estimates
(9) Remaining materials (natural isotopes): P, S, Cl, Ca,....			Automatic production of data libraries
(10) Remaining long-lived nuclides (τ > 1 year)			
(11) Medium long-lived nuclides (1000 sec. ¡ τ < 1 year)	(Almost) no experimental data	Complete reliance on nuclear models, preferably microscopic	(Almost) no integral experimental data
(12) Short-lived nuclides (τ < 1000 sec.)			Astrophysics

D. Rochman and A.J. Koning, TENDL-2011: TALYS-based Evaluated Nuclear Data Library, PHYSOR2012

Essential for (n,γ): Photon strength functions

strength

Model for $E1$ gamma-ray strength function, see Section 10. There are many possibiliti

Examples

strength 1 : Kopecky-Uhl generalized Lorentzian (GLO)
strength 2 : Brink-Axel Lorentzian (SLO)
strength 3 : Hartree-Fock BCS tables
strength 4 : Hartree-Fock-Bogoliubov (HFB) tables
strength 5 : Goriely hybrid model [53]
strength 6 : Goriely T-dependent HFB tables
strength 7 : T-dependent RMF tables
strength 8 : Gogny D1M HFB+QRPA tables
strength 9 : Simplified Modified Lorentian (SMLO) tables
strength 10: Skyrme-BSK27 HFB+QRPA tables
strength 11: D1M-Intra-E1 tables
strength 12: Shellmodel-E1 tables

Range

1 - 12

Default

strength 8

strengthM1

Model for $M1$ gamma-ray strength function. There are various possibilities. For tabulated values, the model numbers are consistent with those for E1.

Examples

strengthM1 1 : Standard Lotentzian with parameters from Eq. (10.15)
strengthM1 2 : Normalize the $M1$ gamma-ray strength function with that of $E1$ as $f_{E1}/(0.0588A^{0.878})$.
strengthM1 3 : Simplified Modified Lorentzian for M1, with spin-flip and scissors mode
strengthM1 4 : RIPL-2 M1 + Kawano Scissors model
strengthM1 8 : Gogny-D1M HFB tables
strengthM1 10: Skyrme-HFB tables
strengthM1 11: D1M-Intra-M1 tables
strengthM1 12: Shellmodel-M1 tables

Range

1, 2, 3, 4, 8, 10, 11, 12

Default

strengthM1=strength for **strength 8, 10, 11 or 12**, **strengthM1 2** for **strength 1 or 2**, and **strengthM1 3** otherwise.

Essential for (n,γ) and all other channels: Level densities

ldmodel

Model for level densities. There are 3 phenomenological level density models and 5 options for microscopic level densities, all described in Chapter 9. It is also possible to choose a level density model per nuclide considered in the reaction.

Examples

ldmodel 1: Constant Temperature + Fermi gas model (CTM)
ldmodel 2: Back-shifted Fermi gas Model (BFM)
ldmodel 3: Generalised Superfluid Model (GSM)
ldmodel 4: Skyrme-Hartree-Fock-Bogolyubov level densities from numerical tables
ldmodel 5: Skyrme-Hartree-Fock-Bogolyubov combinatorial level densities from numerical tables
ldmodel 6: Temperature-dependent Gogny-Hartree-Fock-Bogolyubov combinatorial level densities from numerical tables
ldmodel 7: BSKG3 - Skyrme-Hartree-Fock-Bogolyubov triaxial combinatorial level densities from numerical tables ← Candidate for default
ldmodel 8: QRPA level densities from numerical tables
ldmodel 2 41 93: Back-shifted Fermi gas Model just for this particular nucleus

Range

$1 \leq$ **ldmodel** ≤ 8

Default

ldmodel 1

Goodness-of-fit: Frms with experimental uncertainty

$$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2}$$

Frms = 1.40 means “~40% off”

$$\varepsilon_{rms} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}\ln r_i\right]$$

Erms = 1. means “no model bias”

Instead of

$$r_i = \frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}},$$

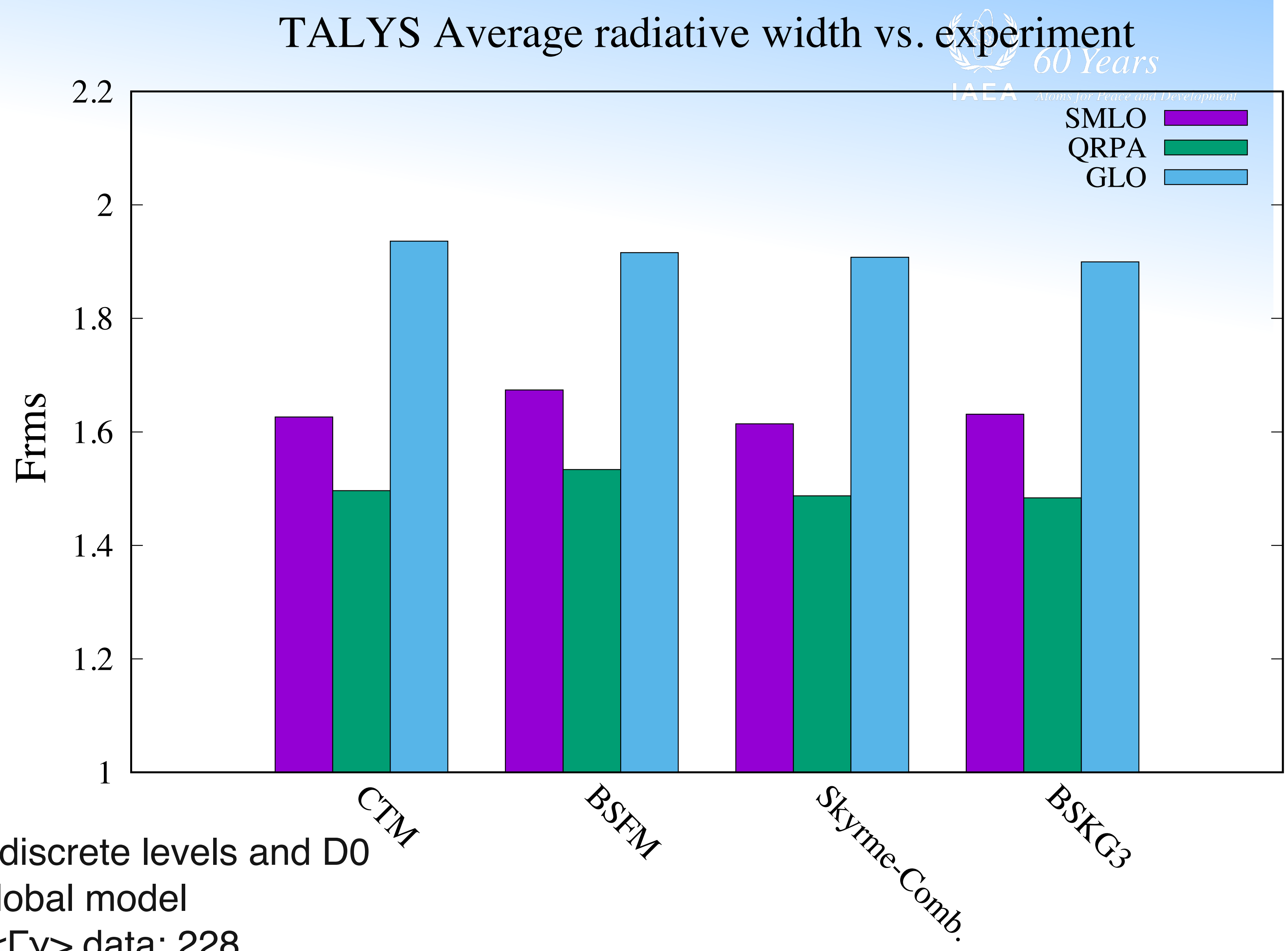
Usual C/E value

we use

$$\begin{aligned} r_i &= 1 - (\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}} - 1)\mathrm{erf}(\frac{x}{\sqrt{2}}) \quad \text{if} \quad \sigma^i_{\rm th} < \sigma^i_{\rm exp}, \\ &= 1 + (\frac{\sigma^i_{\rm th}}{\sigma^i_{\rm exp}} - 1)\mathrm{erf}(\frac{x}{\sqrt{2}}) \quad \text{if} \quad \sigma^i_{\rm th} > \sigma^i_{\rm exp}, \\ &= 1 \quad \text{if} \quad \sigma^i_{\rm th} = \sigma^i_{\rm exp}. \end{aligned}$$

C/E value including uncertainties

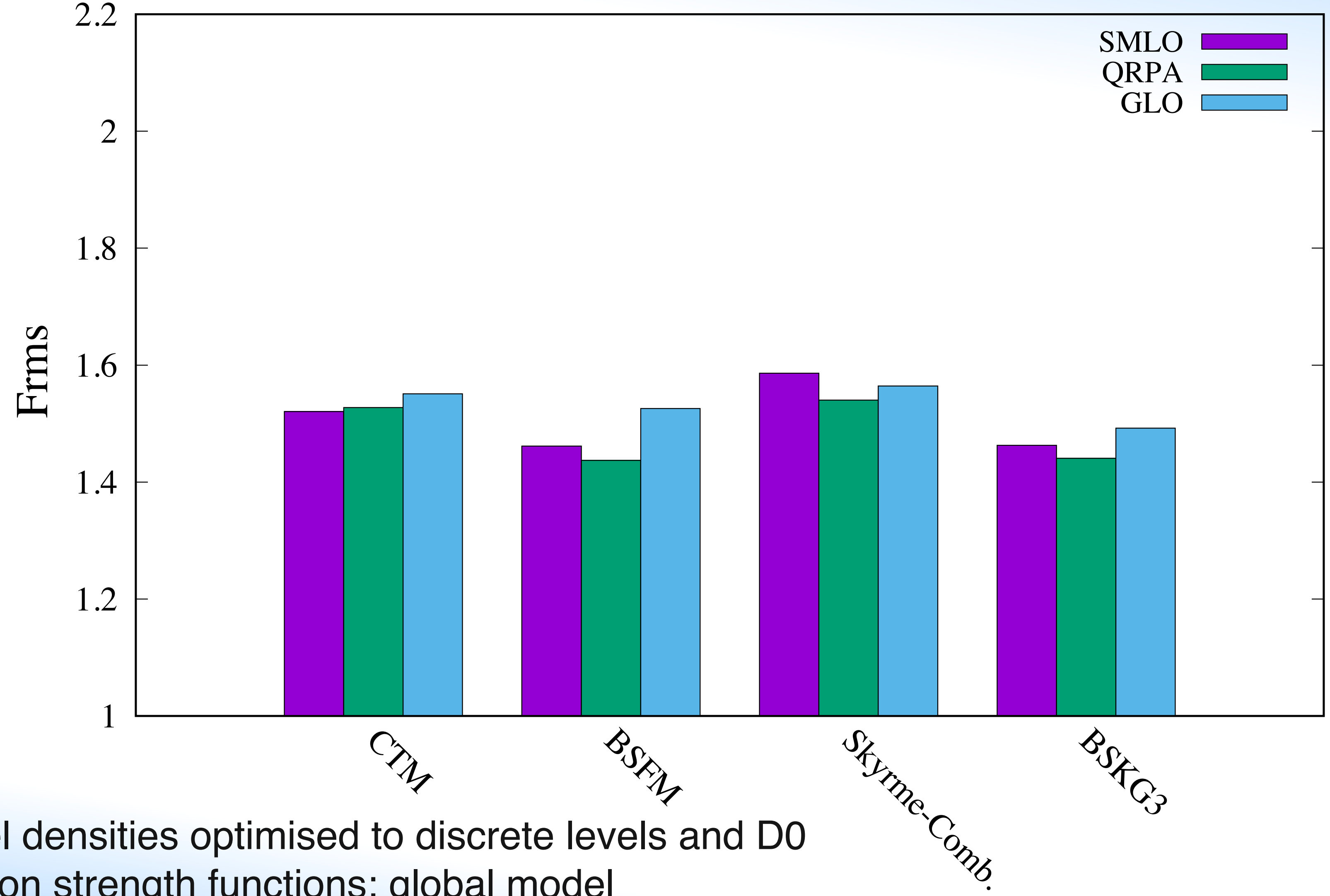
$$x = \frac{\sigma^i_{\rm th} - \sigma^i_{\rm exp}}{\delta\sigma^i_{\rm exp}}$$



Level densities optimised to discrete levels and D0
Photon strength functions: global model
Nuclides with experimental <Γγ> data: 228

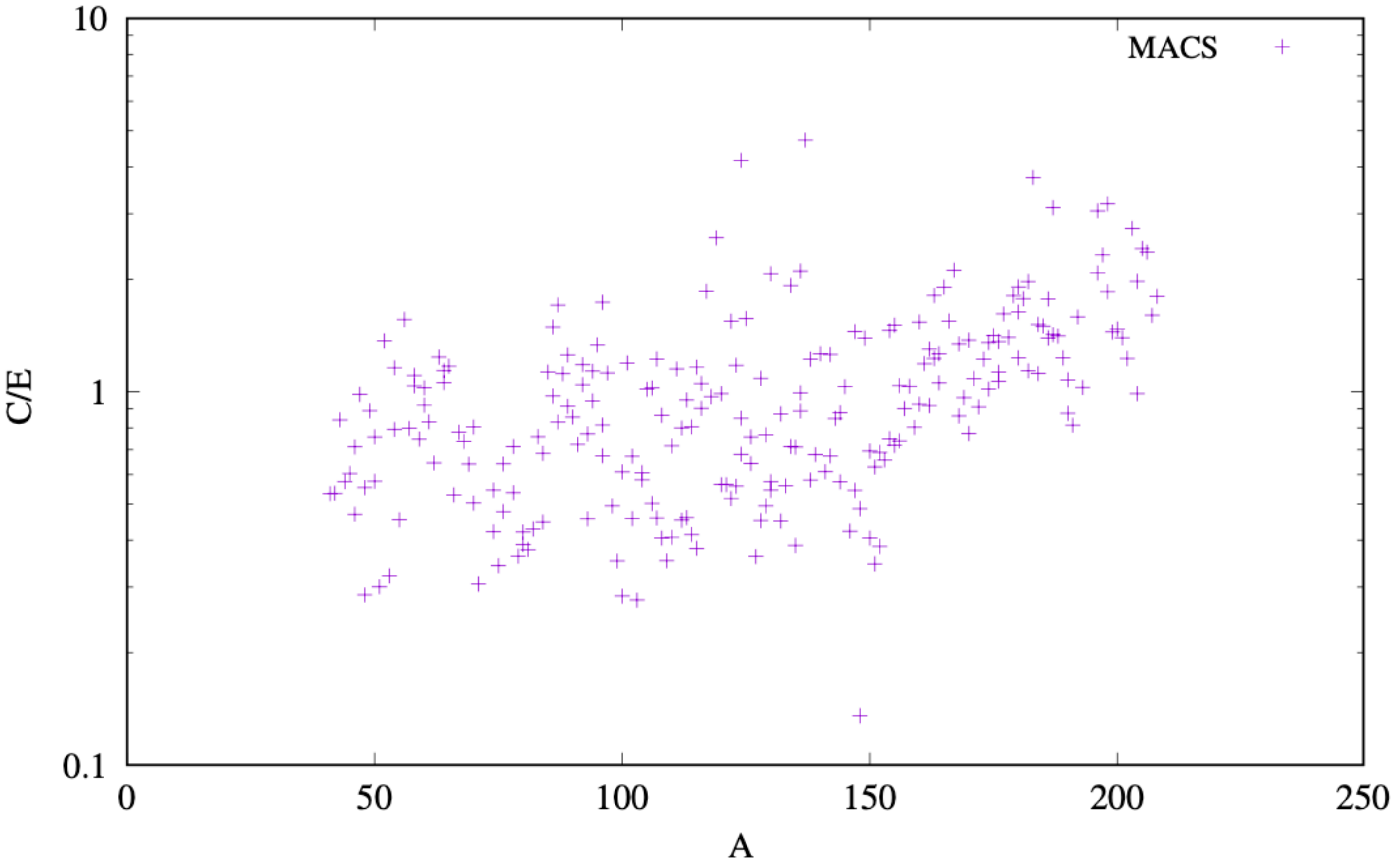
$$\langle\Gamma_\gamma\rangle = \frac{D_0}{2\pi}\sum_{X,L,J,\pi}\int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma)\times\rho(S_n+E_n-\varepsilon_\gamma,J,\pi)d\varepsilon_\gamma$$

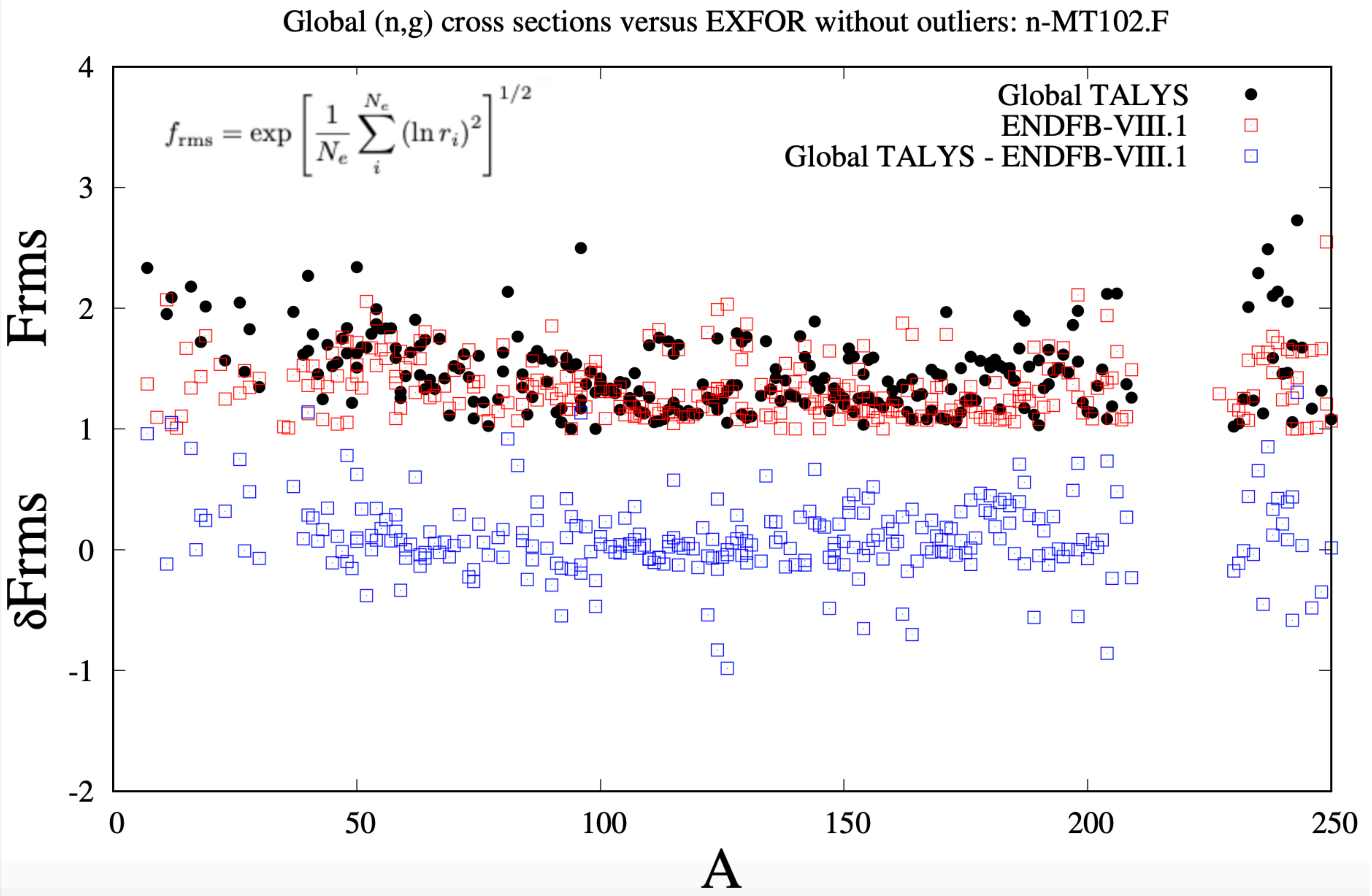
TALYS Maxwellian Averaged cross sections vs. experiment



Level densities optimised to discrete levels and D0
Photon strength functions: global model
Nuclides with experimental MACS data: 277

Global TALYS vs. Experimental data

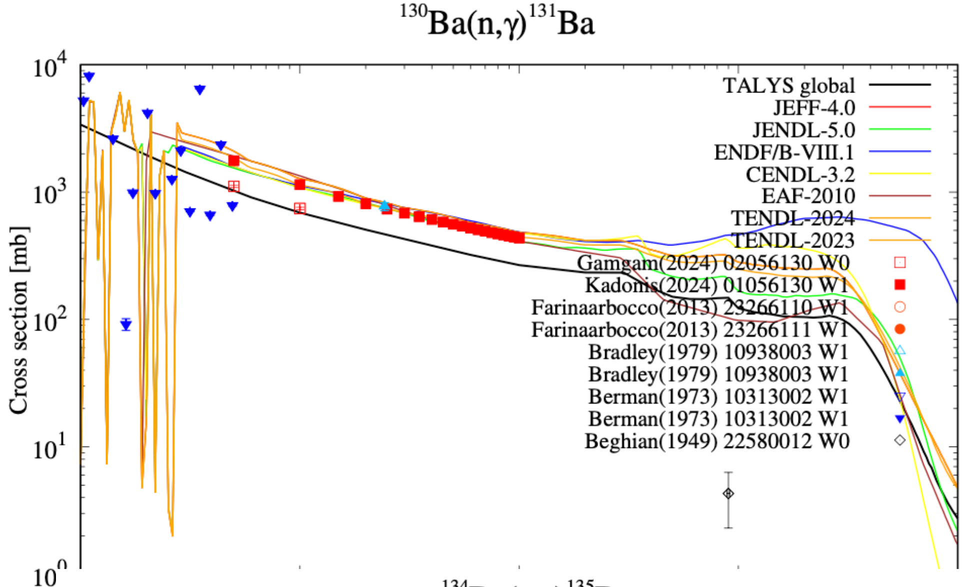


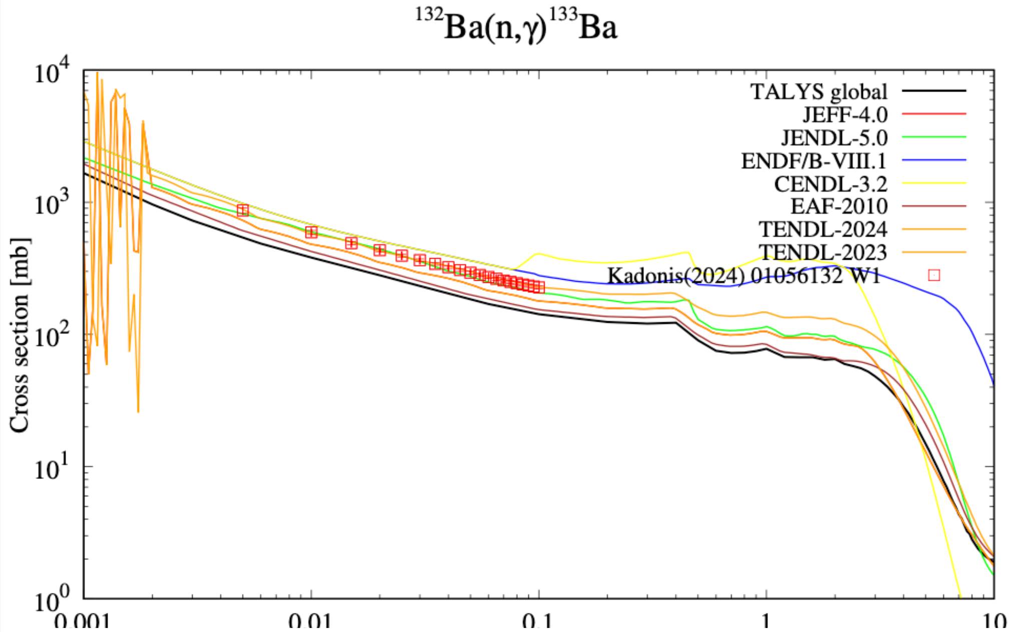


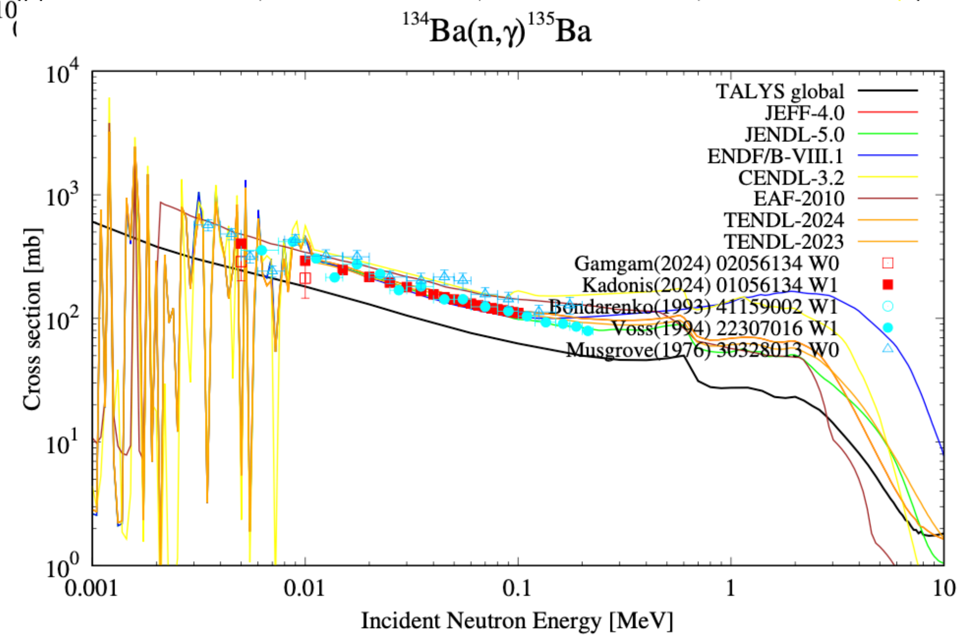
Global (n,g) cross sections versus EXFOR without outliers: n-MT102.F
$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_i^{N_e}(\ln r_i)^2\right]^{1/2}$
Global TALYS
ENDFB-VIII.1
Global TALYS - ENDFB-VIII.1
Frms
δFrms
A
4
3
2
1
0
-1
-2
0
50
100
150
200
250

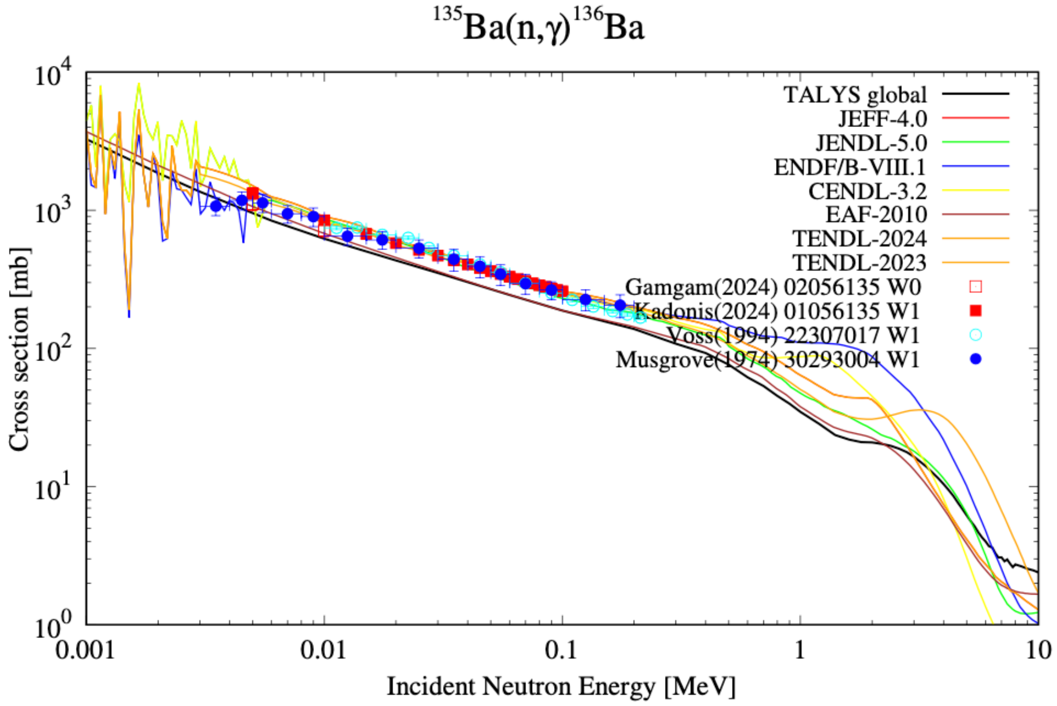
Global (n,γ) : Ba isotopes

MACS unfolded to pseudo cross section data

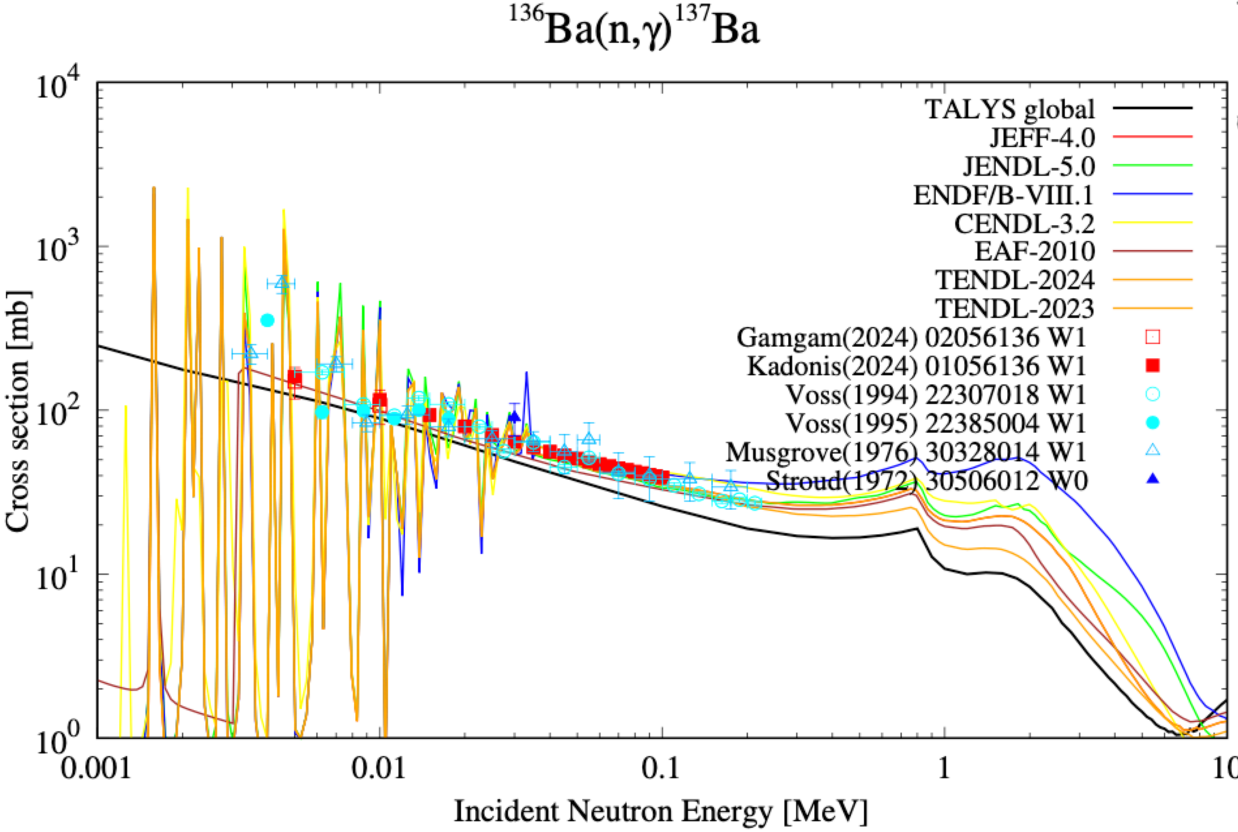


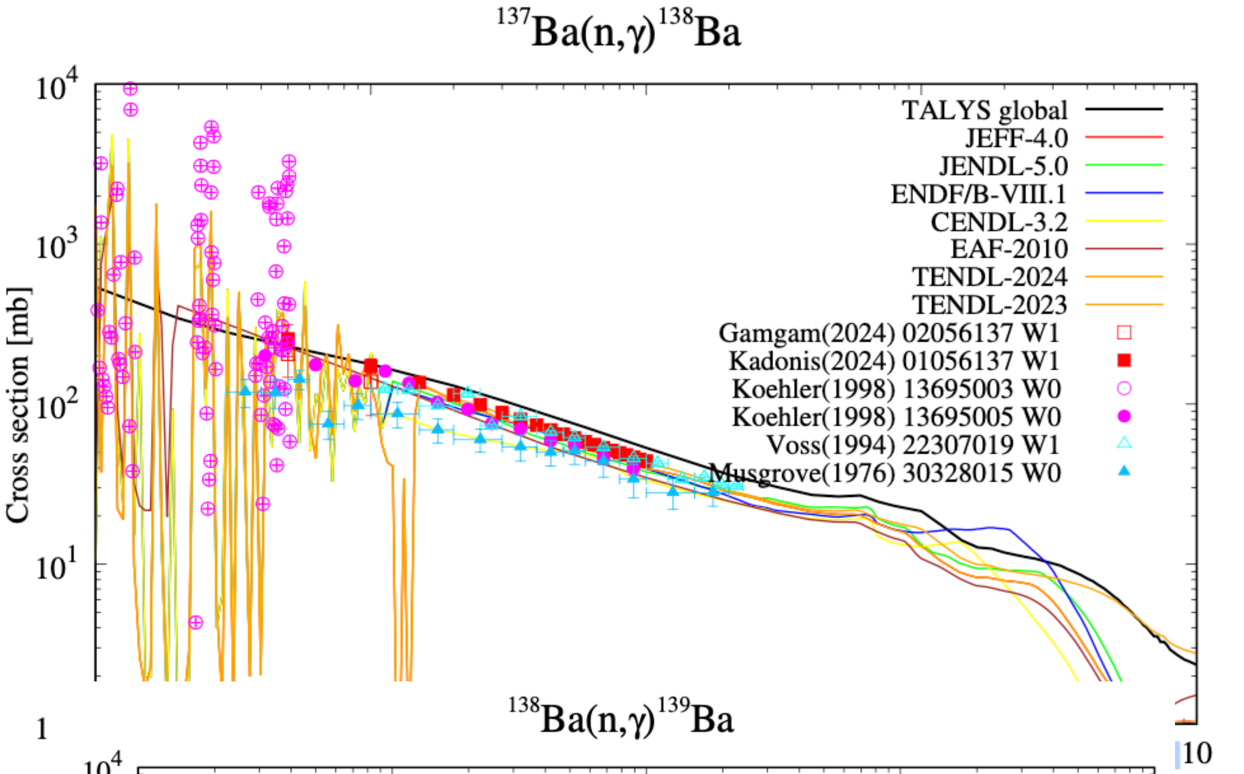


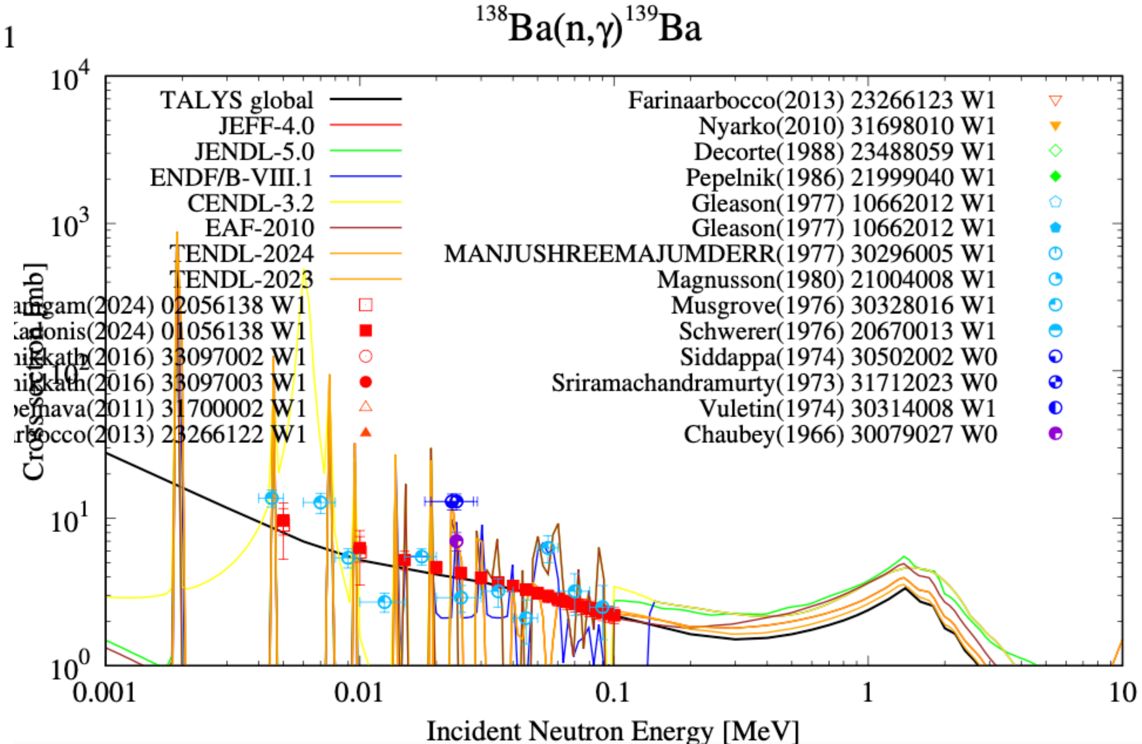




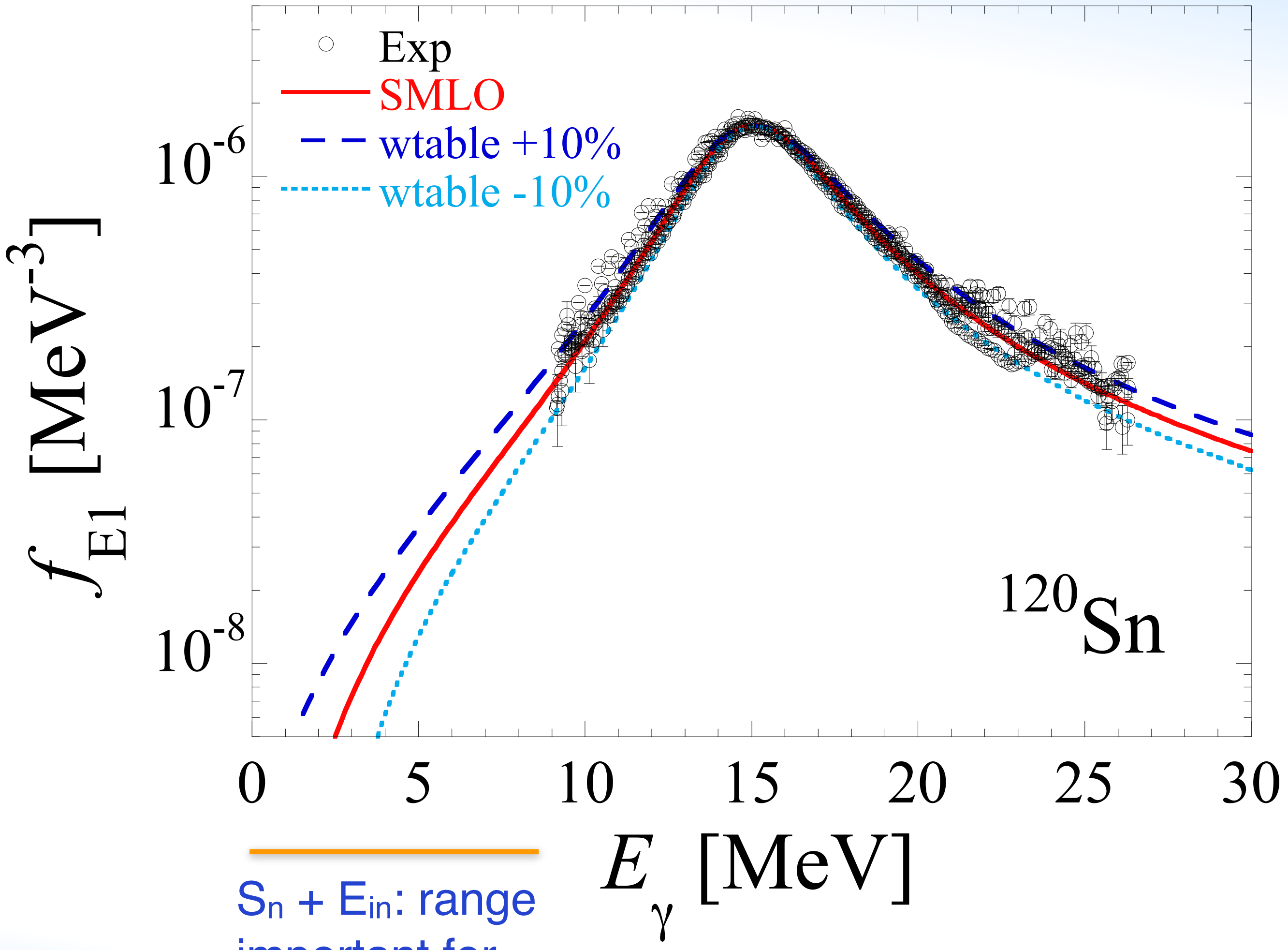
Global (n,γ) : Ba isotopes







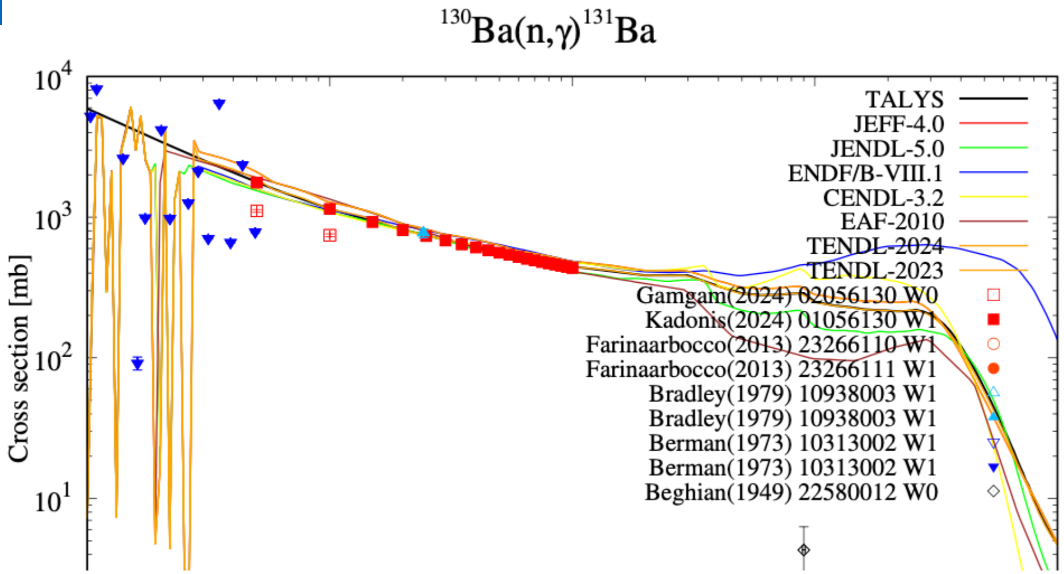
Adjusting (n,γ) cross sections with PSF width parameter

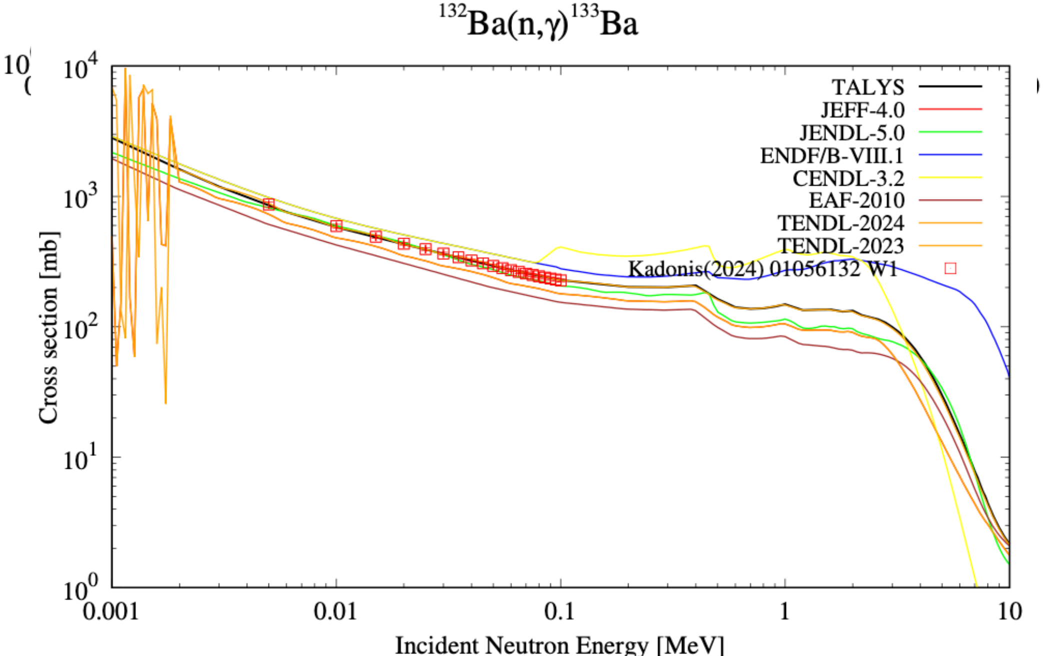


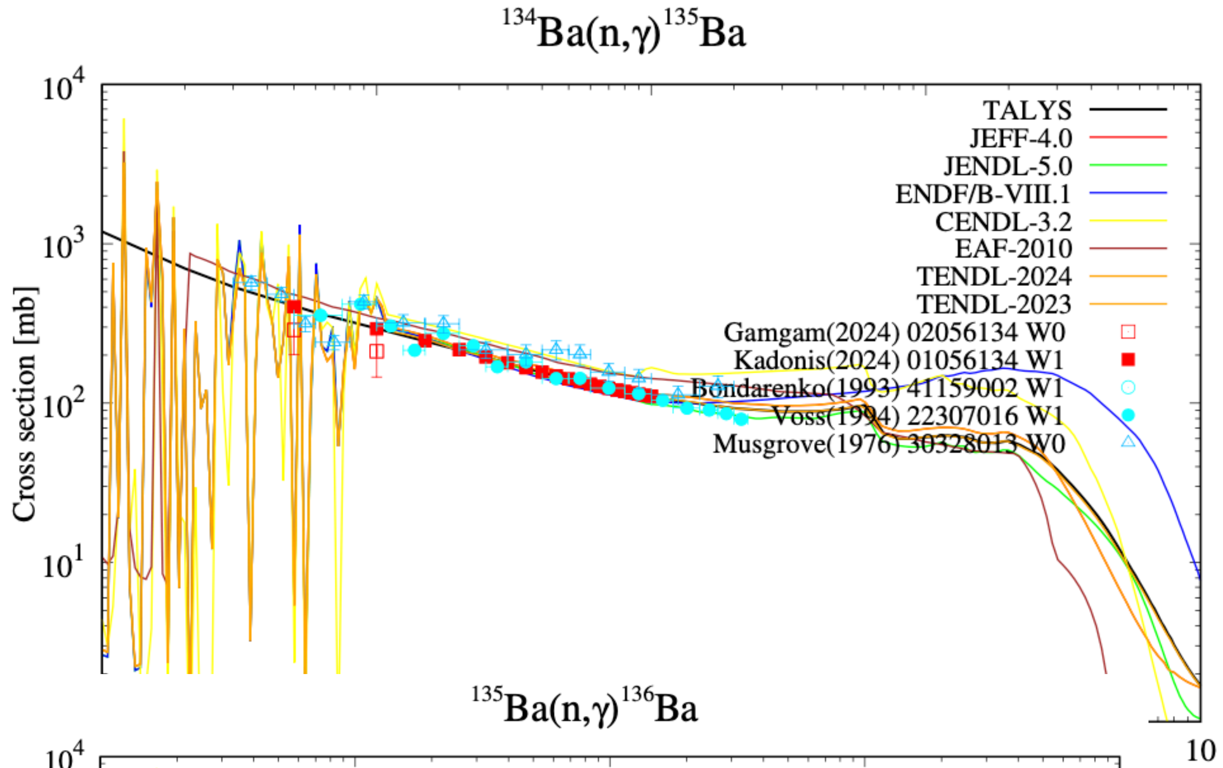
$S_n + E_{in}$: range important for (n,γ)

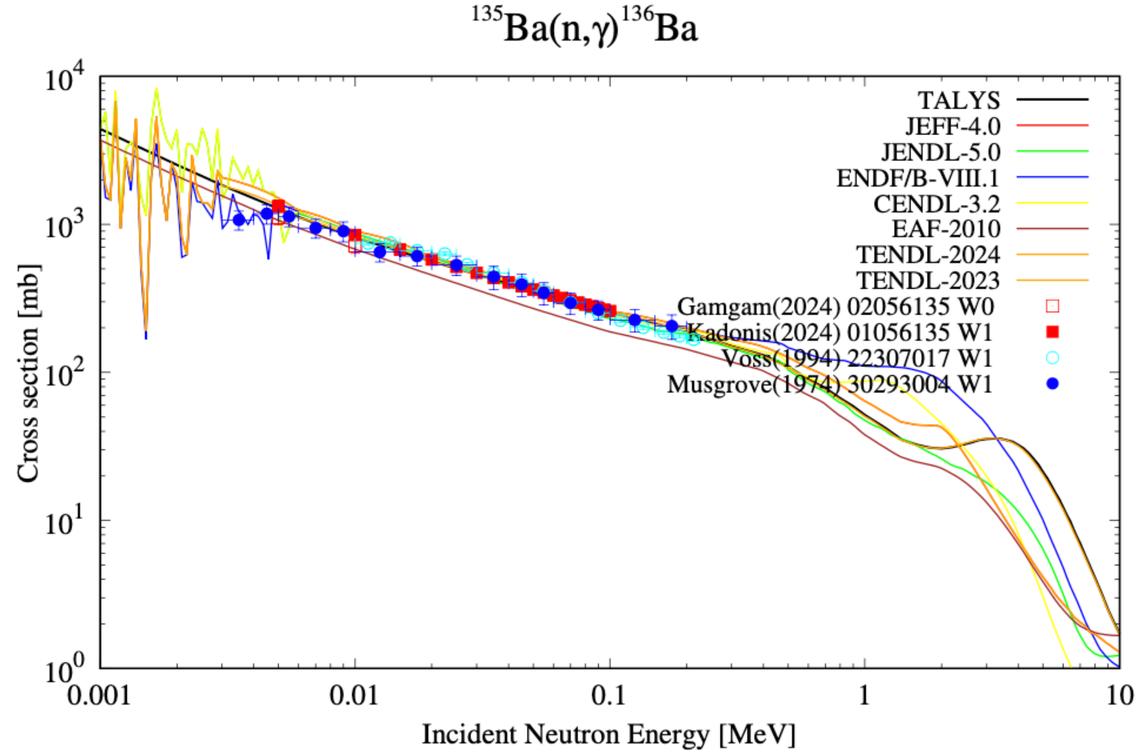
$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$

Optimised (n,γ) : Ba isotopes

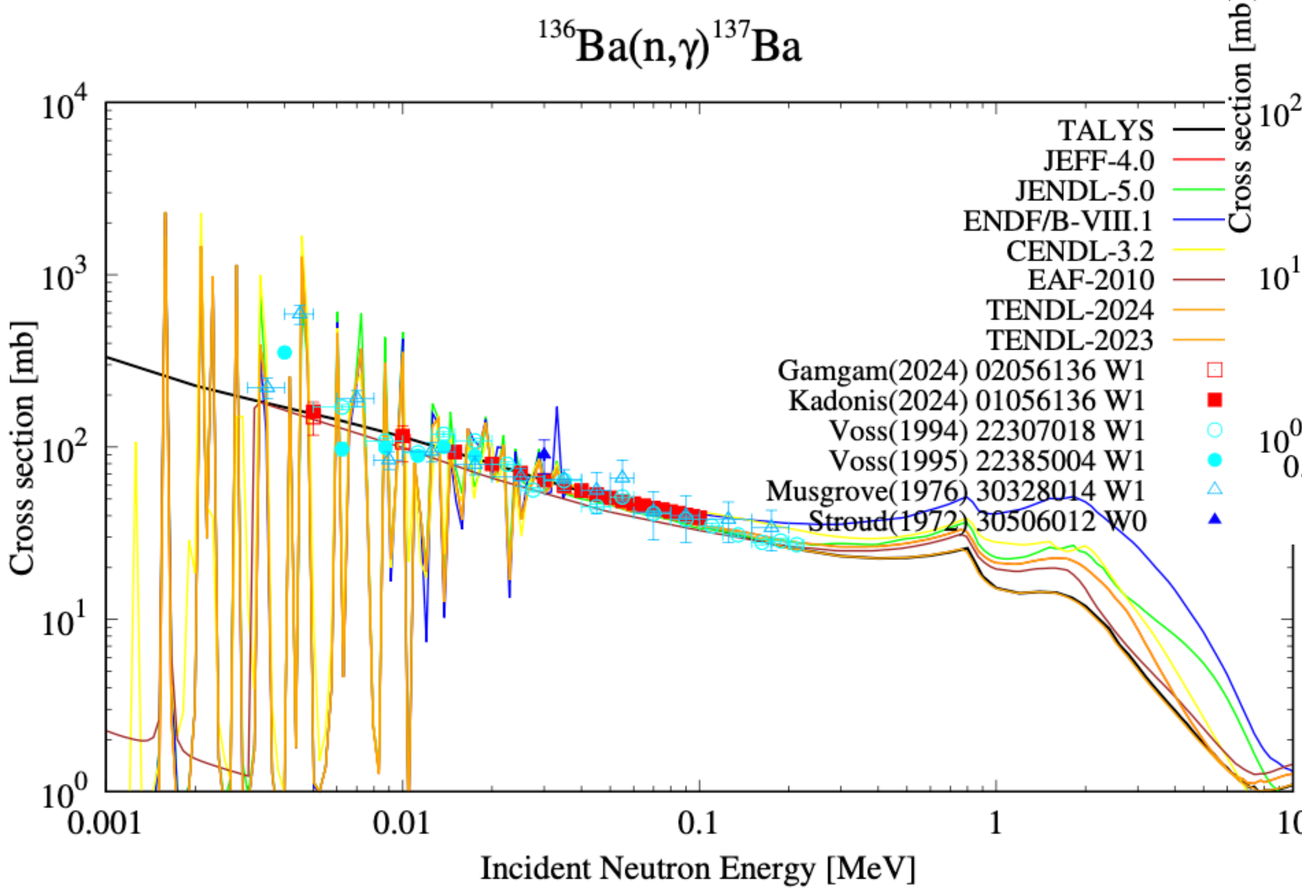


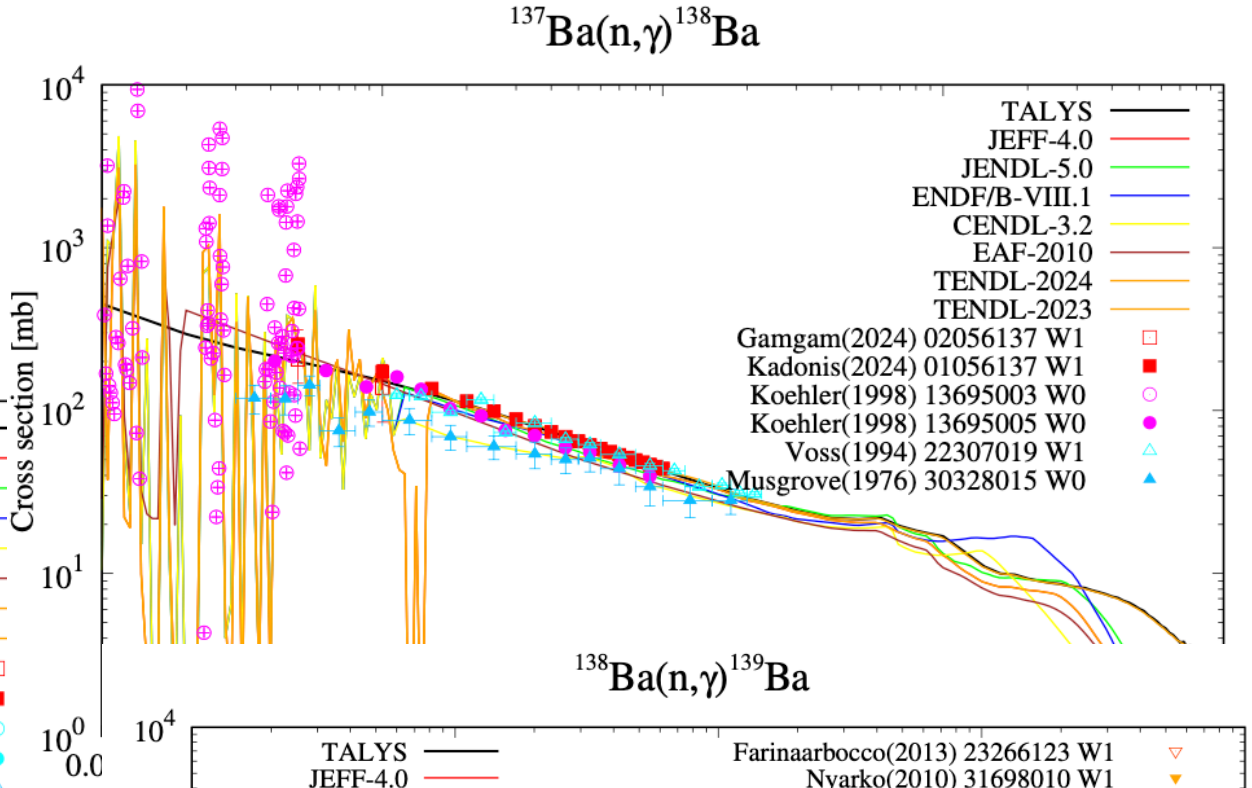


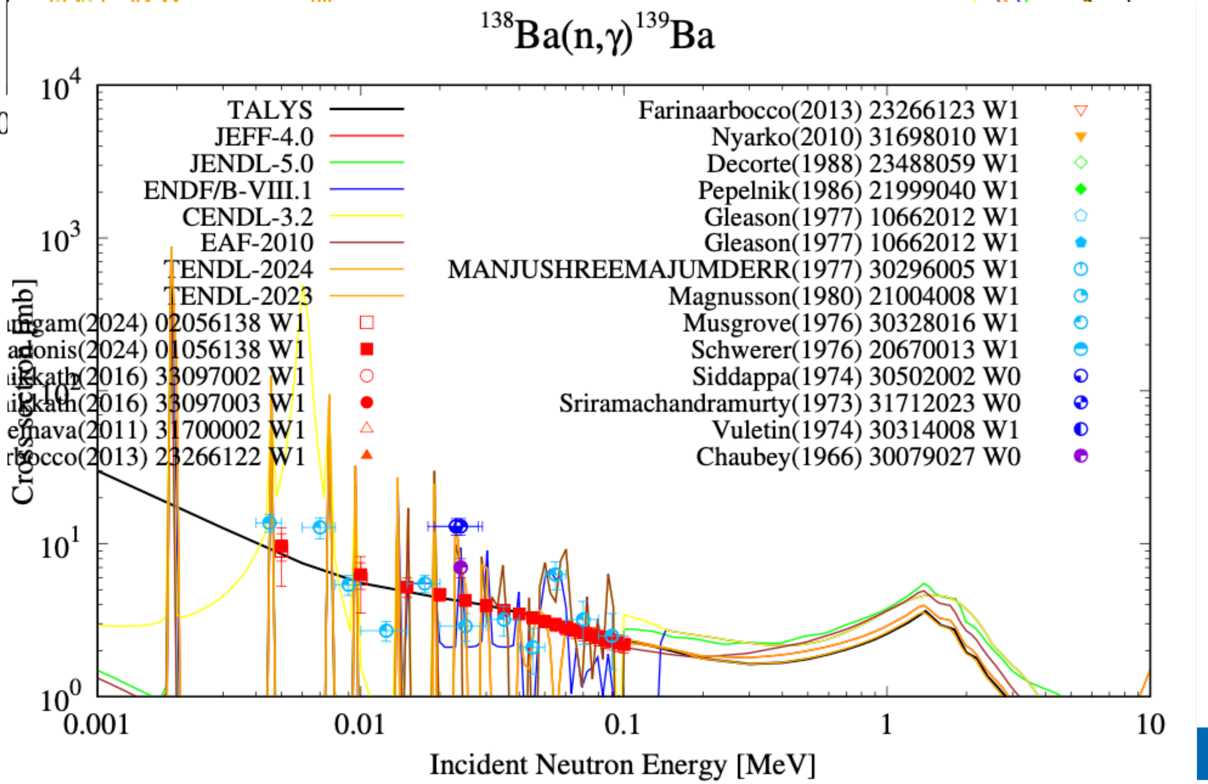




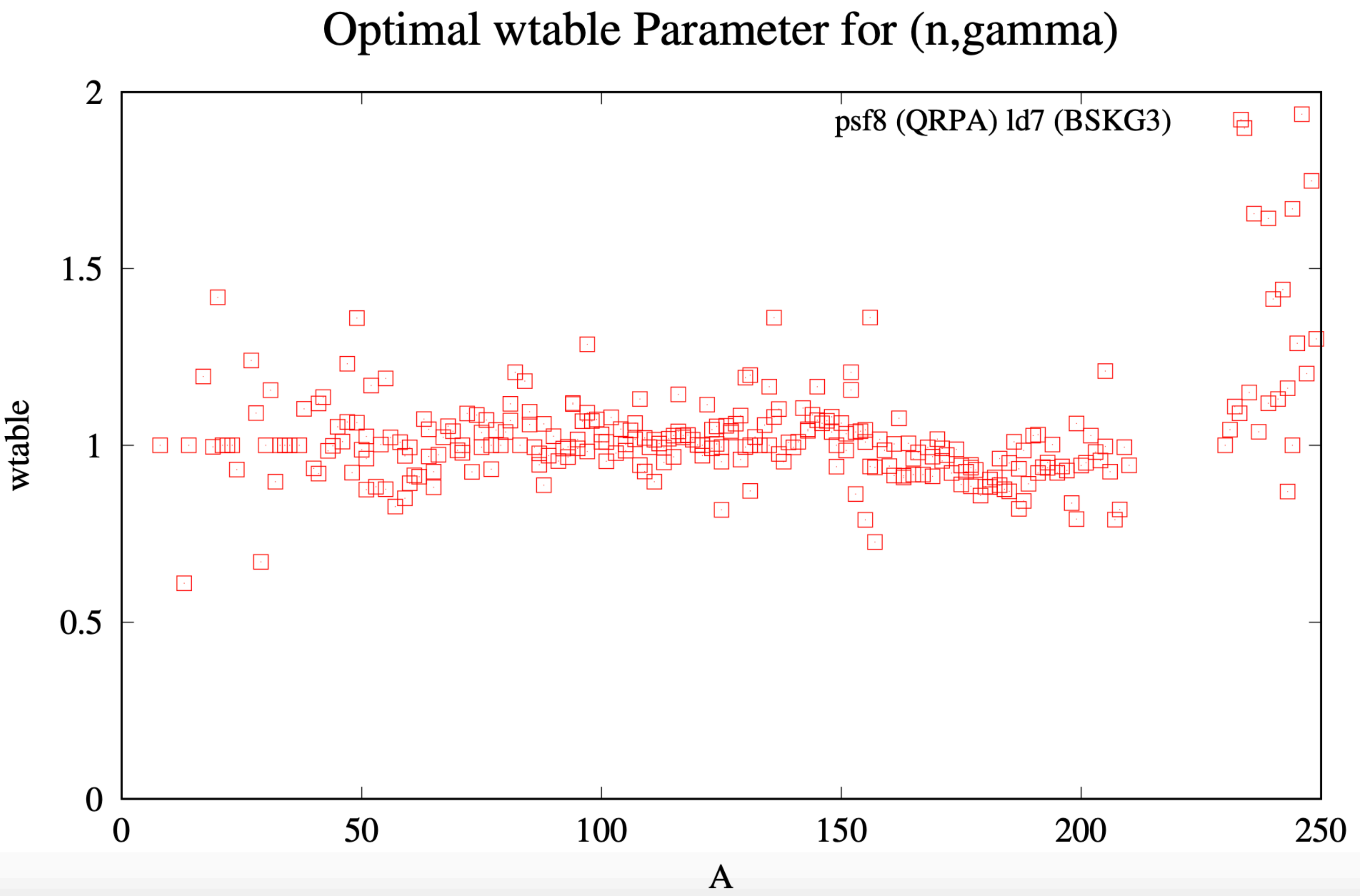
Optimised (n,γ) : Ba isotopes



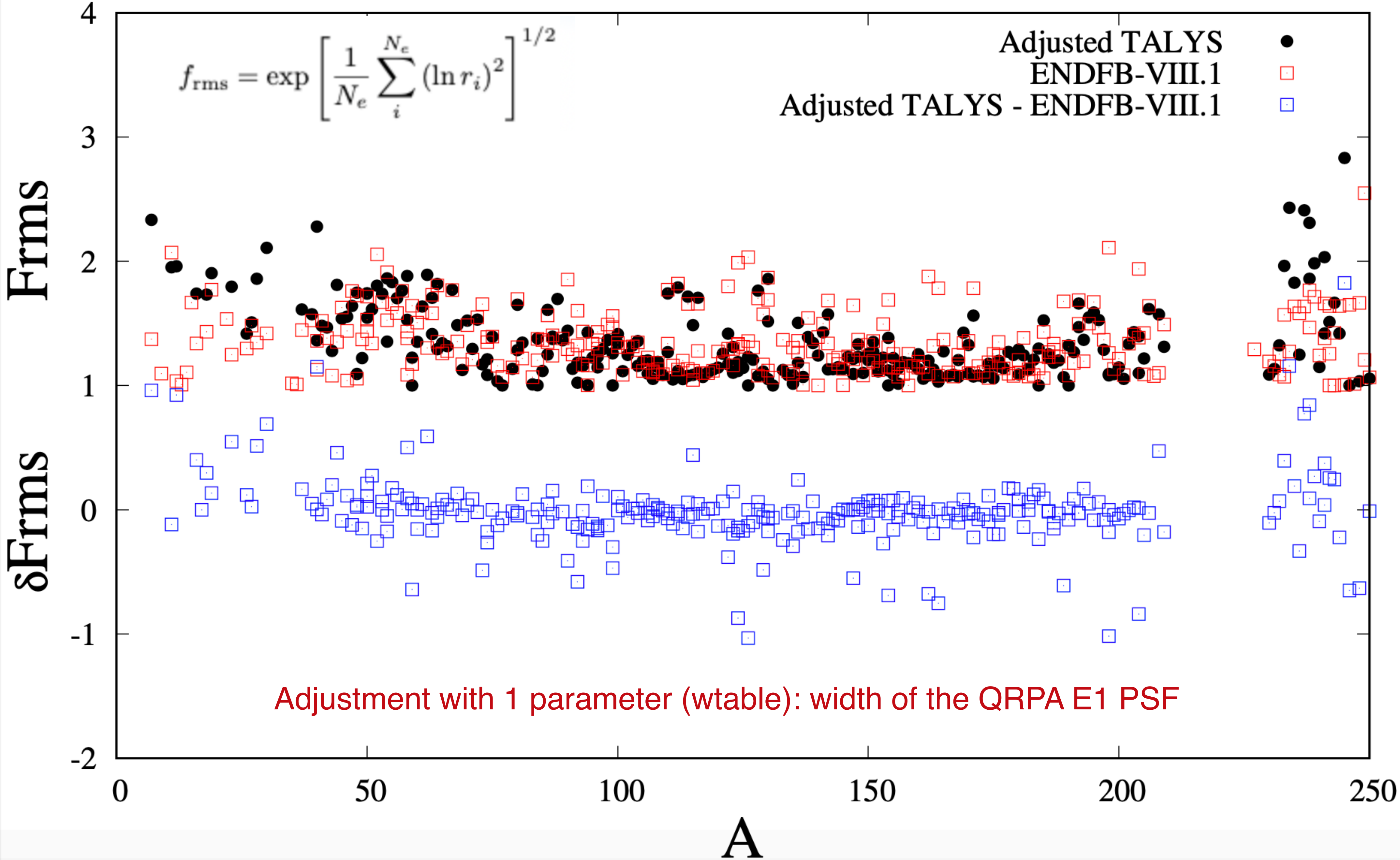




Simultaneous adjustment to MACS, <Γγ> and (n,γ) cross sections



Adjusted (n,g) cross sections versus EXFOR without outliers: n-MT102.F



Adjustment with 1 parameter (wtable): width of the QRPA E1 PSF

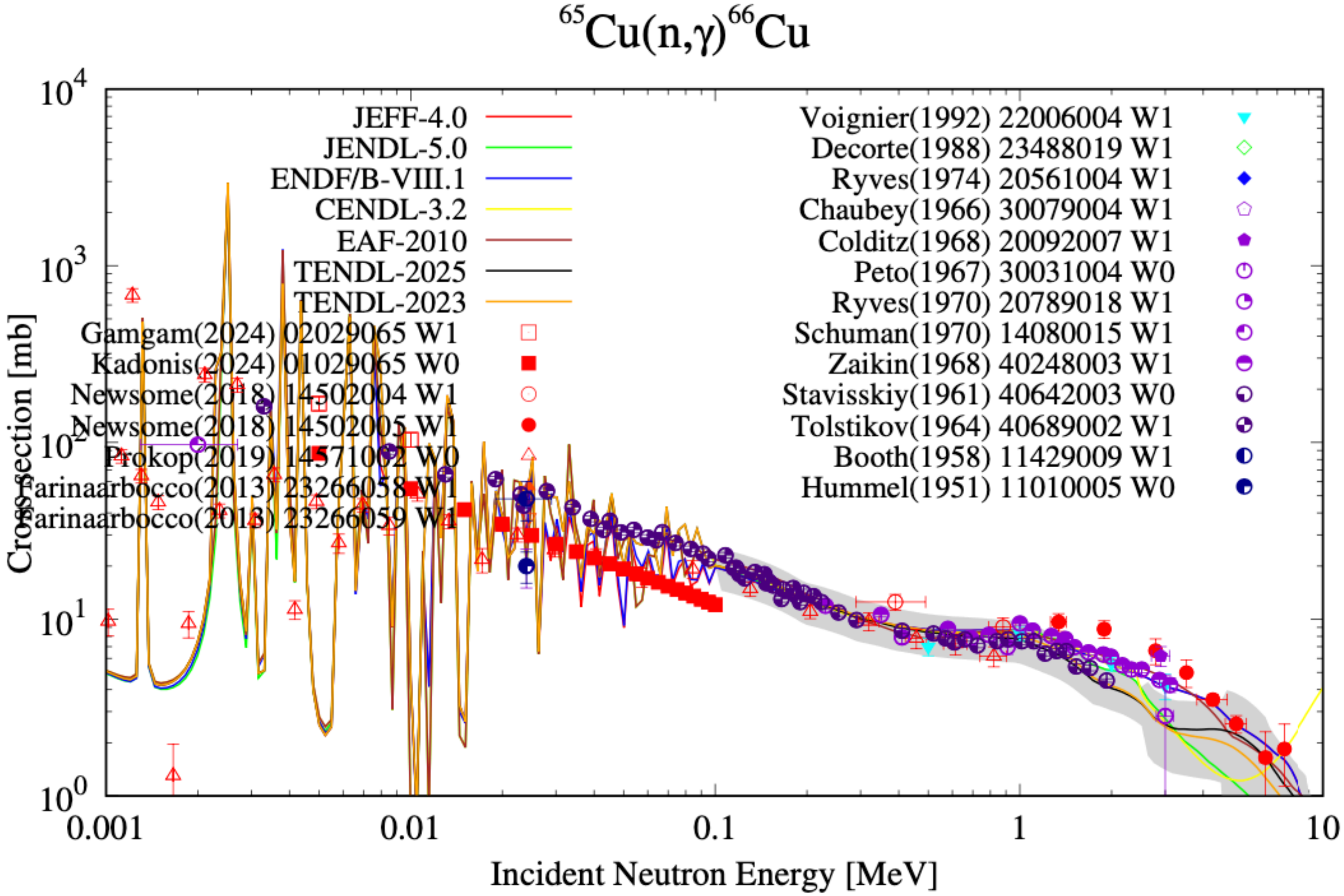
Maxwellian-Averaged Cross Section (MACS)

- In general: consistent with experimental data for average radiative width $\Gamma\gamma$ and ‘normal’ cross section measurements
- Global rule for this work: Astral > Kadonis > Bao et al > Mughabghab > Sukhoruchkin > EXFOR (to be judged/ overruled by real experts!)
- Exceptions:
  - Cu63: Bao et al
  - Cu65: Bao et al
  - Br81: Bao et al
  - Cd106: Mughabghab Atlas 2018
  - Cd108: Sukhoruchkin Atlas 2012
  - Sm148: Kadonis
  - Sm154: Sukhoruchkin
- Any database should clearly distinguish experimental values from the rest
- EXFOR data mining so far: Tm171(Guerrero), W185(Mohr), Th232(Poenitz), U235,238 (Wallner) in EXFOR but not in Astral/Kadonis/Bao

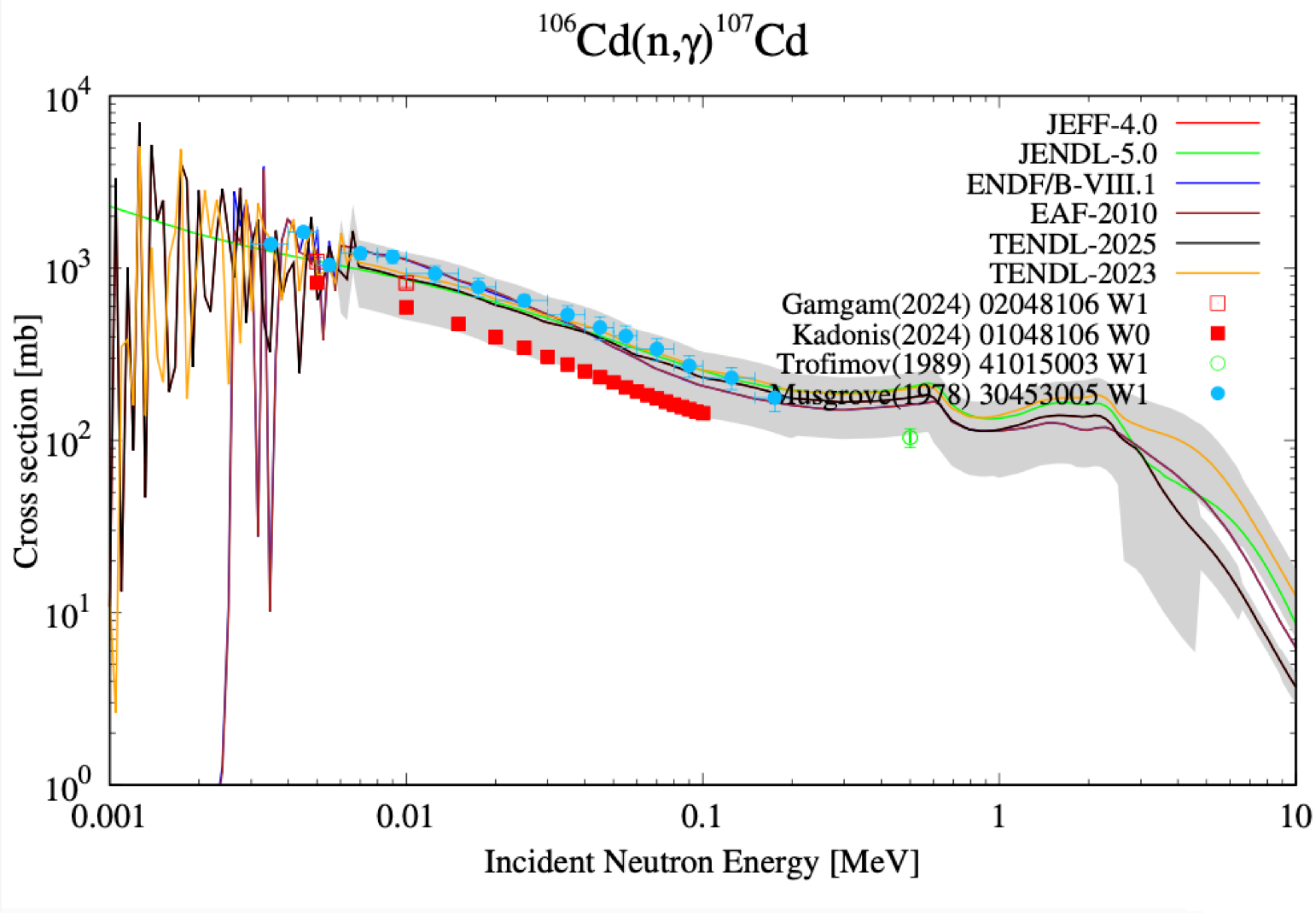
Use all MACS sources we can find

```
# header:
#   title: Ba136(n,g) MACS
#   source: Resonancetables
#   date: 2025-08-25
# target:
#   Z: 56
#   A: 136
#   nuclide: Ba136
# reaction:
#   type: (n,g)
# observables:
#   selected value [b]:  6.739025E-02
#   selected value uncertainty [b]:  2.259080E-03
#   selected value source: Astral
#   number of values: 12
#   average value [b]:  6.742585E-02
#   relative standard deviation [%]:     11.017920
# quantity:
#   type: Compilation spectrum-averaged
#   average value:  6.485806E-02
#   relative standard deviation [%]:      5.329576
# datablock:
#   columns: 11
#   entries: 5
##    Author                        Type          Year          Value         dValue        Reference        Ratio        Spectrum        Energy
##      []             []            []            []           [b]           [b]            []              []            []            [MeV]
      Bao                     Compilation       2000      6.120000E-02  2.000000E-03                  0.908143   MXW           3.000000E-02
      Kadonis                 Compilation       2010      6.120000E-02  2.000000E-03                  0.908143   MXW           3.000000E-02
      Sukhoruchkin            Compilation       2015      7.000000E-02  1.100000E-02                  1.038726   MXW           3.000000E-02
      Mughabghab-2018         Compilation       2018      6.450000E-02  2.100000E-03                  0.957112   MXW           3.000000E-02
      Astral                  Compilation       2020      6.739025E-02  2.259080E-03                  1.000000   MXW           3.000000E-02
# quantity:
#   type: EXFOR
#   average value:  9.000000E-02
#   relative standard deviation [%]:      0.000000
# datablock:
#   columns: 11
#   entries: 1
##    Author                        Type          Year          Value         dValue        Reference        Ratio        Spectrum        Energy
##      []             []            []            []           [b]           [b]            []              []            []            [MeV]
      Stroud                  EXFOR             1972      9.000000E-02  2.000000E-02  30506012        1.335505                 3.000000E-02
# quantity:
#   type: EXFOR spectrum-averaged
#   average value:  6.200000E-02
#   relative standard deviation [%]:      0.000000
# datablock:
#   columns: 11
#   entries: 1
##    Author                        Type          Year          Value         dValue        Reference        Ratio        Spectrum        Energy
##      []             []            []            []           [b]           [b]            []              []            []            [MeV]
      Wisshak                 EXFOR             1994      6.200000E-02  2.100000E-03  22337004        0.920014   MXW           3.000000E-02
# quantity:
#   type: Nuclear data library
#   average value:  6.656400E-02
#   relative standard deviation [%]:      3.478802
# datablock:
#   columns: 11
#   entries: 5
##    Author                        Type          Year          Value         dValue        Reference        Ratio        Spectrum        Energy
##      []             []            []            []           [b]           [b]            []              []            []            [MeV]
      cendl3.2                NDL               2019      6.776800E-02  0.000000E+00                  1.005605   MXW           3.000000E-02
      jendl5.0                NDL               2021      6.621700E-02  0.000000E+00                  0.982590   MXW           3.000000E-02
      endfb8.1                NDL               2024      7.022900E-02  0.000000E+00                  1.042124   MXW           3.000000E-02
      tendl.2025              NDL               2025      6.519300E-02  0.000000E+00                  0.967395   MXW           3.000000E-02
      jeff4.0                 NDL               2025      6.341300E-02  0.000000E+00                  0.940982   MXW           3.000000E-02
```

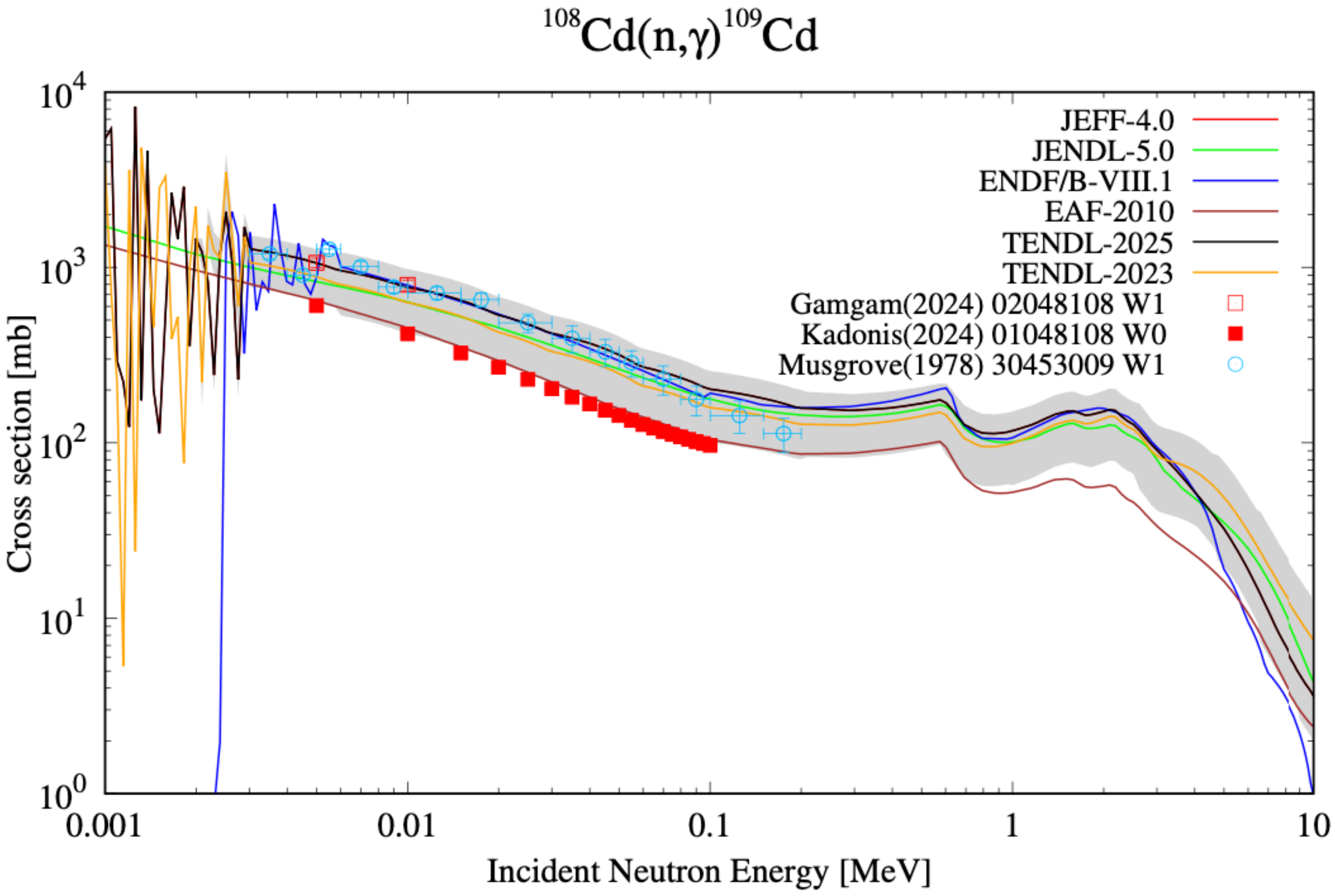
Outlier: Cu65



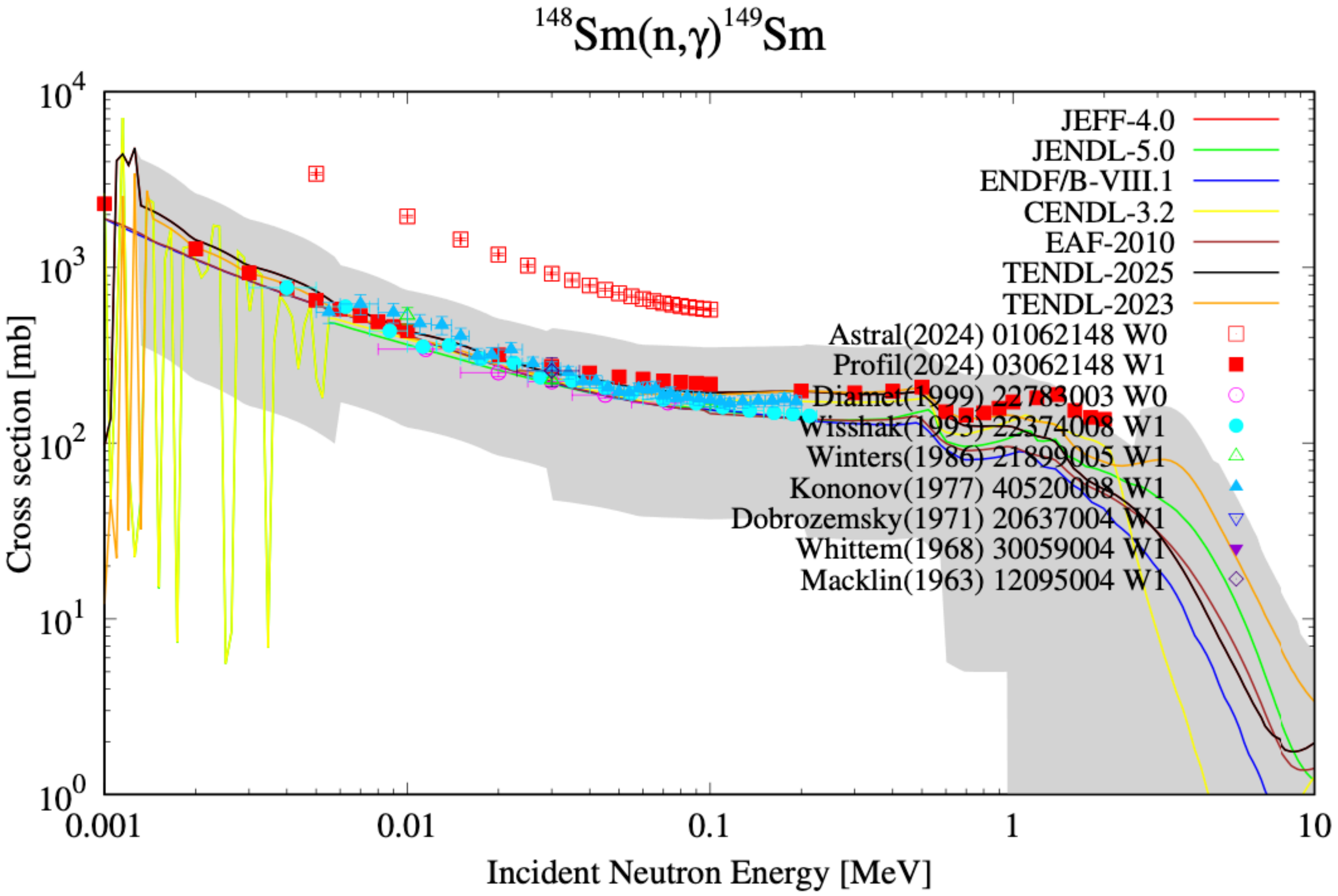
Outlier: Cd106



Outlier: Cd108



Outlier: Sm148



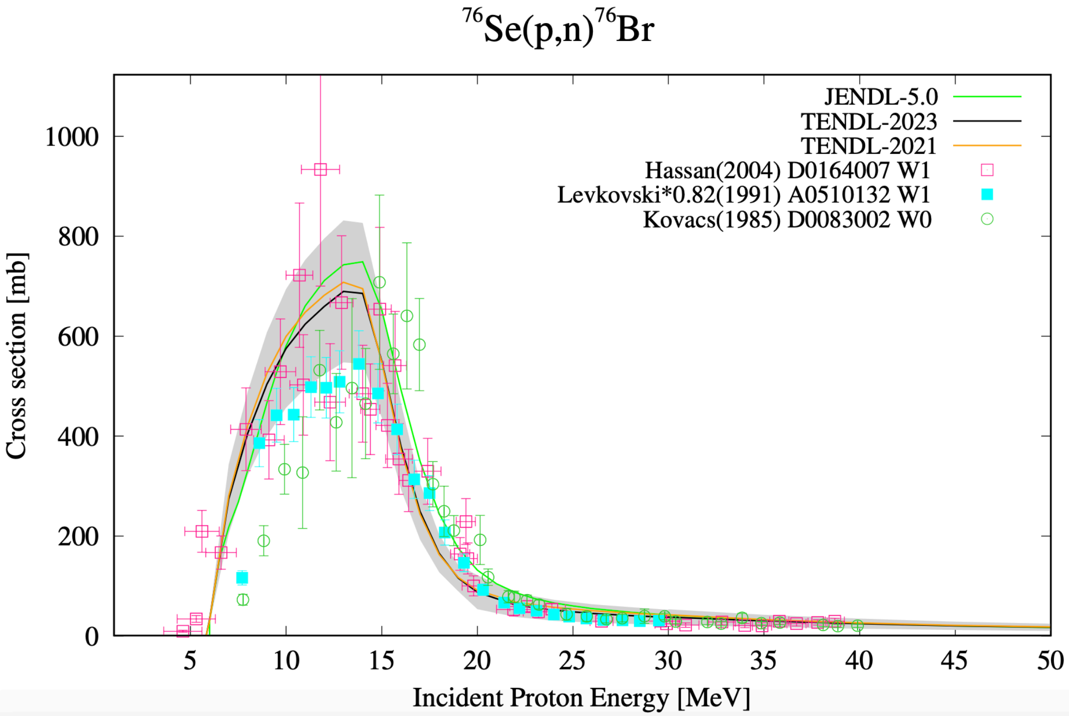
Experimental data

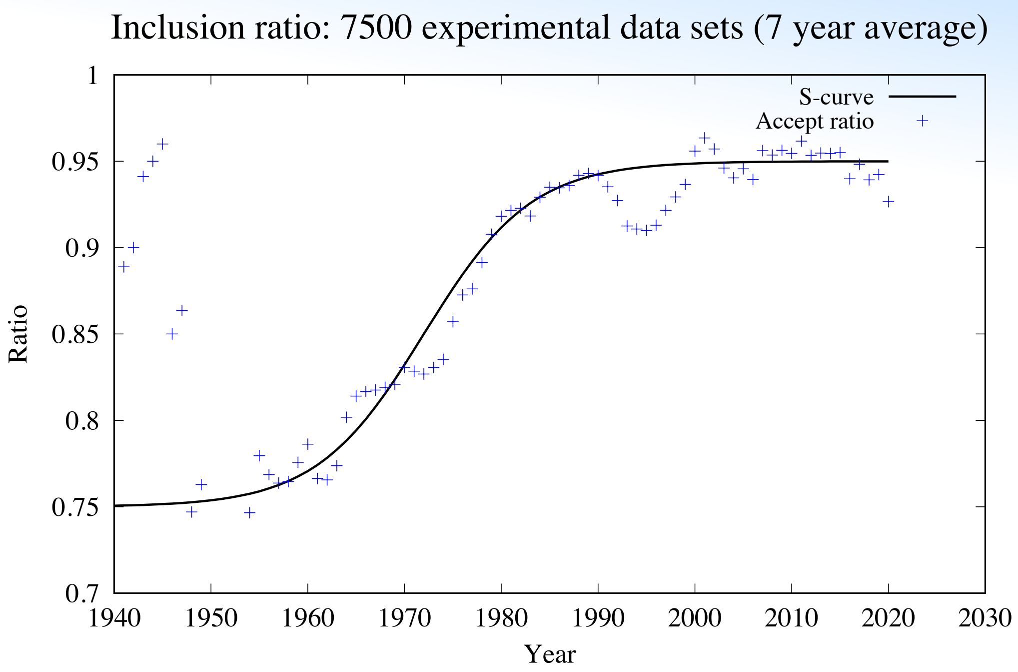
- TALYS/TENDL methodology requires **all** EXFOR to be available instantaneously
- Best current option: EXFORtables - directory structured database
- All data normalised to latest standards/monitors
- Outlier assignment:
  - 23444 cross section data sets
  - 10969 declared inlier
  - 1975 declared outlier
  - Still need to put 23444 JSON files on IAEA-github

EXFORCISM: flag evil experimental data sets as outlier

Koning, Dzysiuk, Alhassan, Gaughan
Now 13 000 data sets for neutrons up to alpha particles. Cross sections only.
Outliers based on comparison with other exp. data, NDL's and TALYS:

- Visual,
- Rms goodness-of-fit
- reading papers (Dzysiuk, Alhassan)





Essential for automated parameter optimisation with TALYS

For our horizontal data evaluation:
~1960: 25% of exp. data sets not included
> 2000: 5% of exp. data sets not included

60 Years

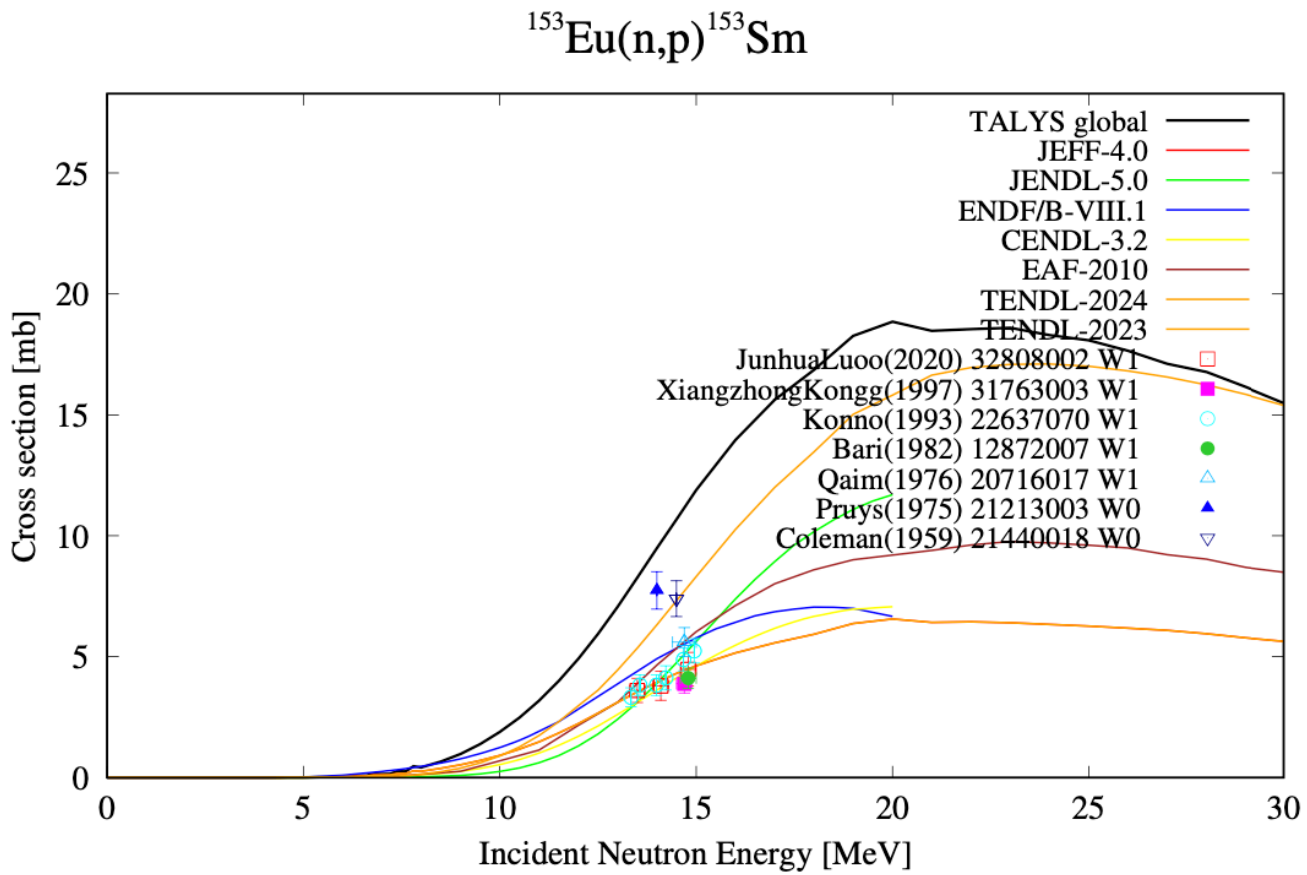
Atoms for Peace and Development

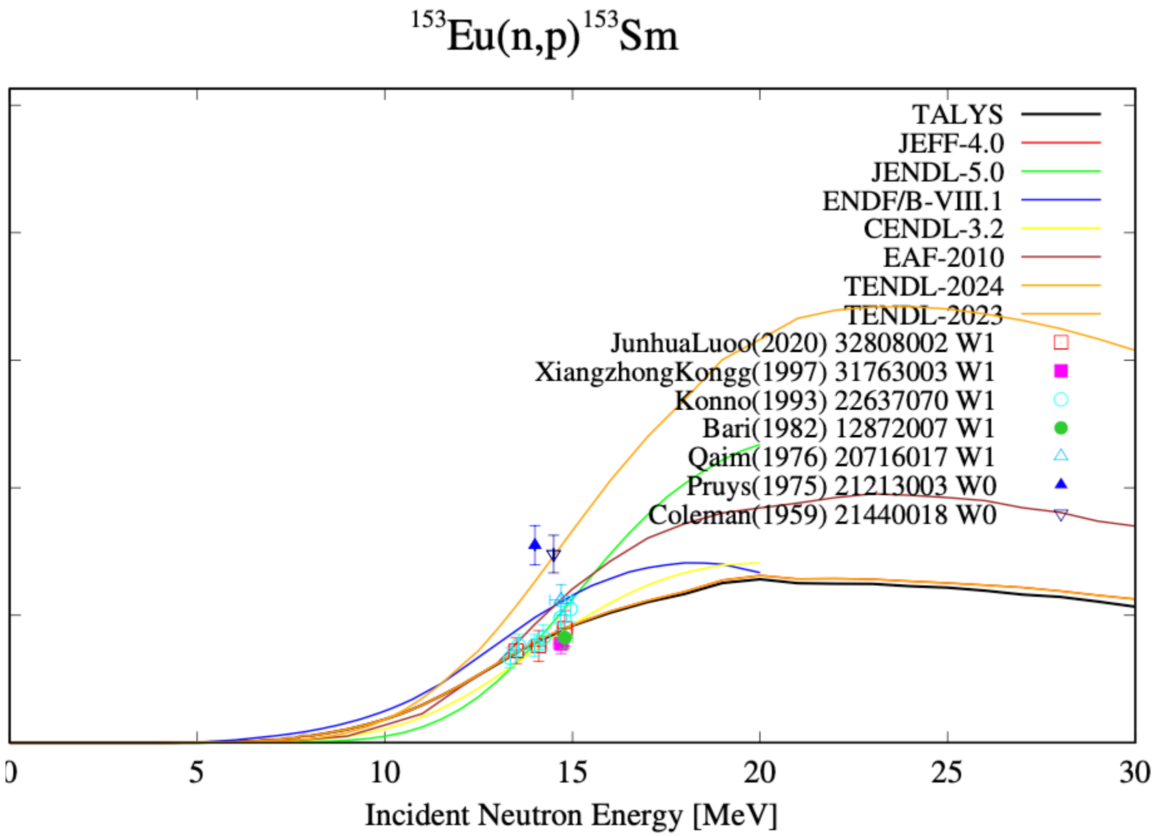

```
/Users/koning/quality/json> cat 12033007.json
{
    "Subentry"    : "12033007",
    "Author"      : "Wille",
    "Year "       : 1960,
    "Projectile"  : "n",
    "Target Z"    :   57,
    "Target A"    :  139,
    "Target state": "0",
    "Reaction"    : "(n,x)",
    "Final Z"     :   55,
    "Final A"     :  136,
    "Final state" : "g",
    "Quantity"    : "Cross section",
    "X4 Reaction" : "57-LA-139(N,A)55-CS-136-G,,SIG",
    "MF"          :    3,
    "MT"          :  107,
    "Evaluations" :
    [
        {
        "Evaluator"   : "Arjan Koning",
        "Date"        : "2022-12-13",
        "Weight"      :    0,
        "Comment"     : [
                        " Excluded from evaluation: graphical outlier"
                        ]
        },
        {
        "Evaluator"   : "Arjan Koning (2020)",
        "Date"        : "2012-06-30",
        "Weight"      :   -1,
        "Comment"     : [
                        "NEA quality score: R2"
                        ]
        },
        {
        "Evaluator"   : "Natalia Dzysiuk (2018)",
        "Date"        : "2018-03-24",
        "Weight"      :    0,
        "Comment"     : [
                        " wrong half-life, inconsistent time of irradiation"
                        ]
        }
    ]
}
```

Parameter optimisation up to 20 MeV

- Use TASMAN code (nds.iaea.org/talys): Either Czendes global optimization based on Boender-Rinnooy-Kan-Timmer-Stougie stochastic method, or Nelder-Mead optimisation
  - Multi-dimensional parameter landscape not too wild
  - 20 TALYS runs per varied parameter usually enough: 120-160 TALYS runs for optimal result
- (n,γ):
  - PSF: wtable(0,0) - width of PSF of compound nucleus
- (n,n’), (n,2n), (n,3n), (n,p) and (n,np):
  - rvadjust p - radius of proton OMP for outgoing channel
  - gadjust(0,0), gadjust(0,1), gadjust(1,0) - particle-hole density for pre-equilibrium
- (n, α)
  - rvadjust a - radius of α OMP for outgoing channel
  - cstrip a - Kalbach parameter for stripping reaction
- Isomer versus ground state:
  - Risomer - discrete level branching ratio of final nuclide
  - s2adjust - level density spin distribution of final nuclide

Global versus optimised





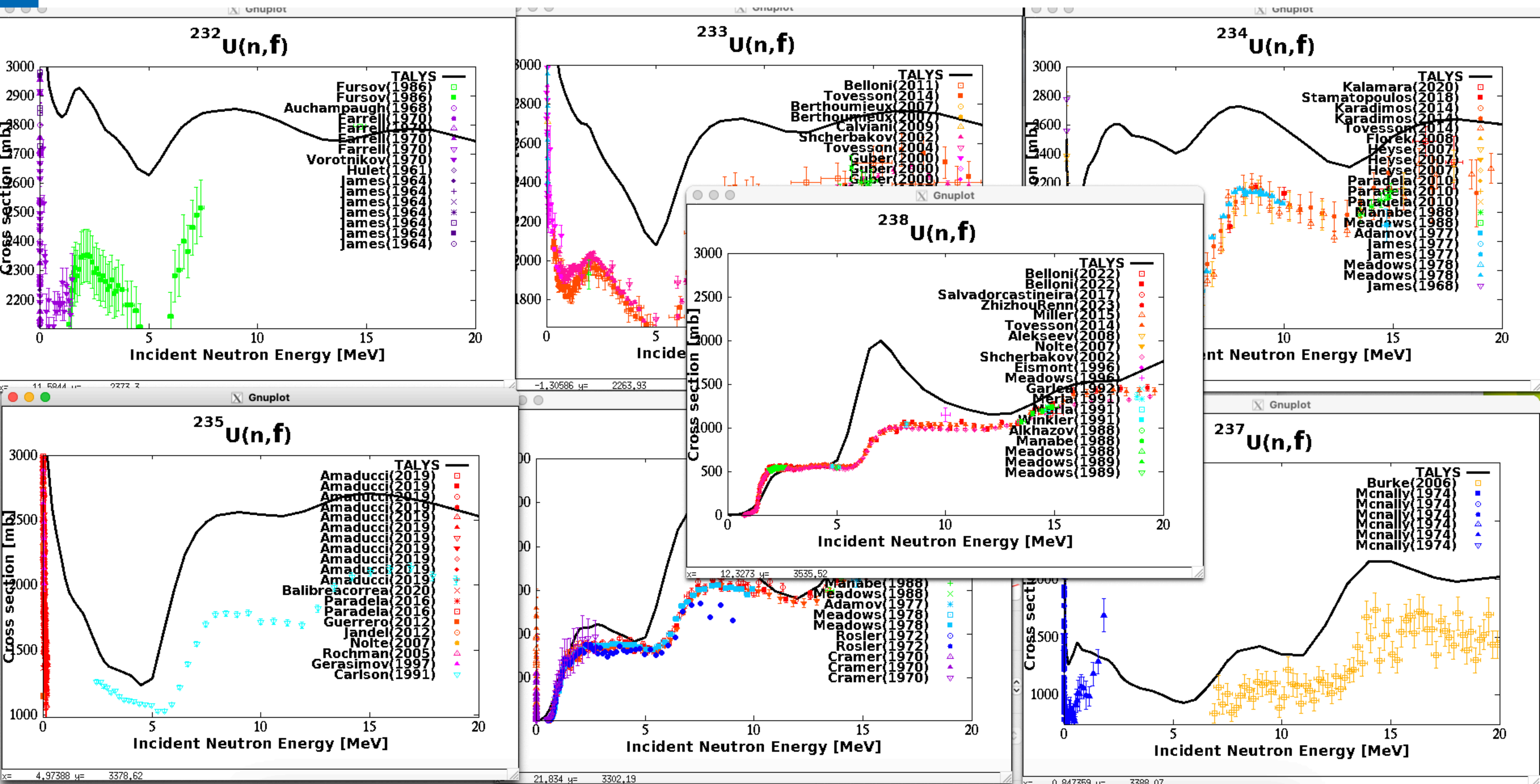
Global calculations for actinides

```
#
# TALYS input file generated by Autotalys
#
projectile n
element    U
mass       235
Ltarget    000
energy     energies
partable y
bins 40
maxrot 5
strength 9
strengthm1 3
upbend y
ldmodel 7
fismodel 6
#fispartdamp y
hbstate n
class2 n
filechannels y
channels y
#
# Set multi-preequilibrium switch lower for actinides
#
multipreeq 20.
#
# Reduce output for activation-only calculation
#
outspectra n
outangle n
ddxmode 0
outdiscrete n
alphaomp 6
riplrisk y
```

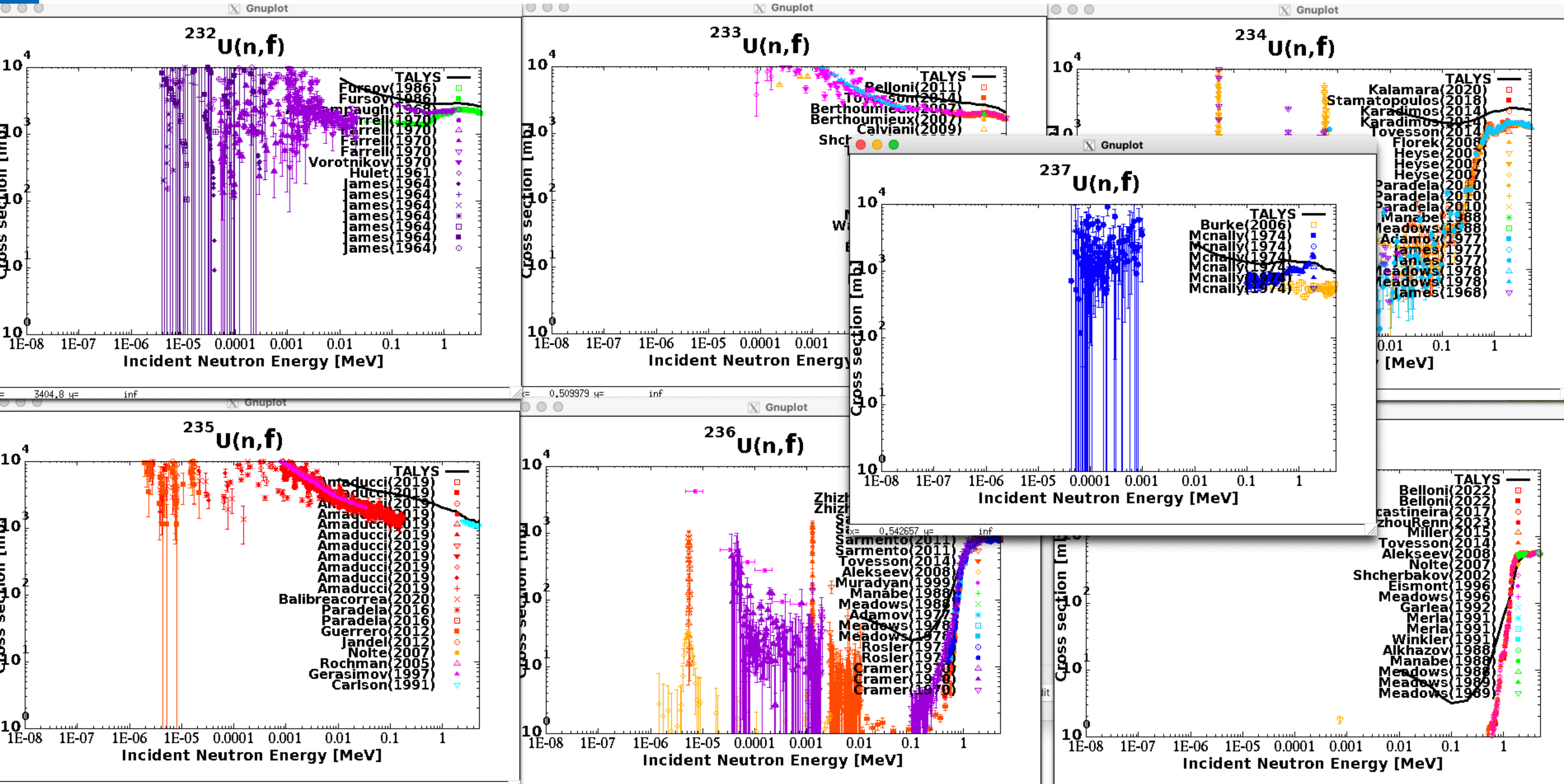
BSKG3 (ldmodel 7, fismodel 6)

Capote et al RIPL 2408 (riplrisk y)

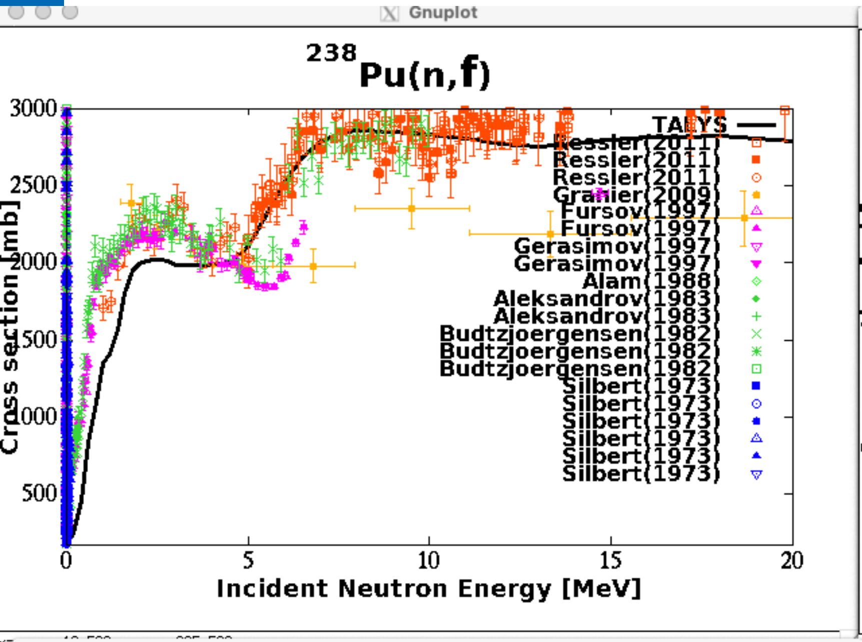
Global calculations for U isotopes

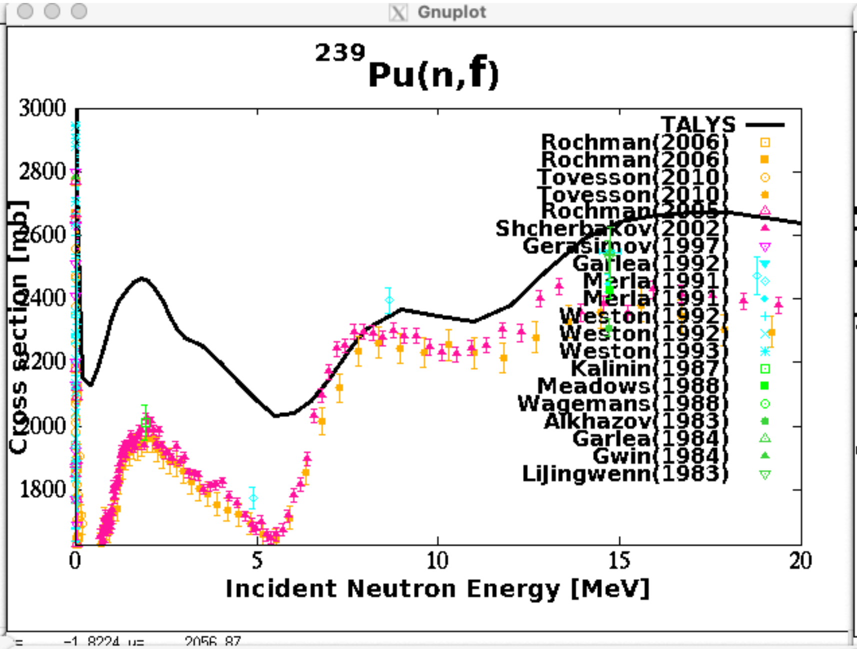


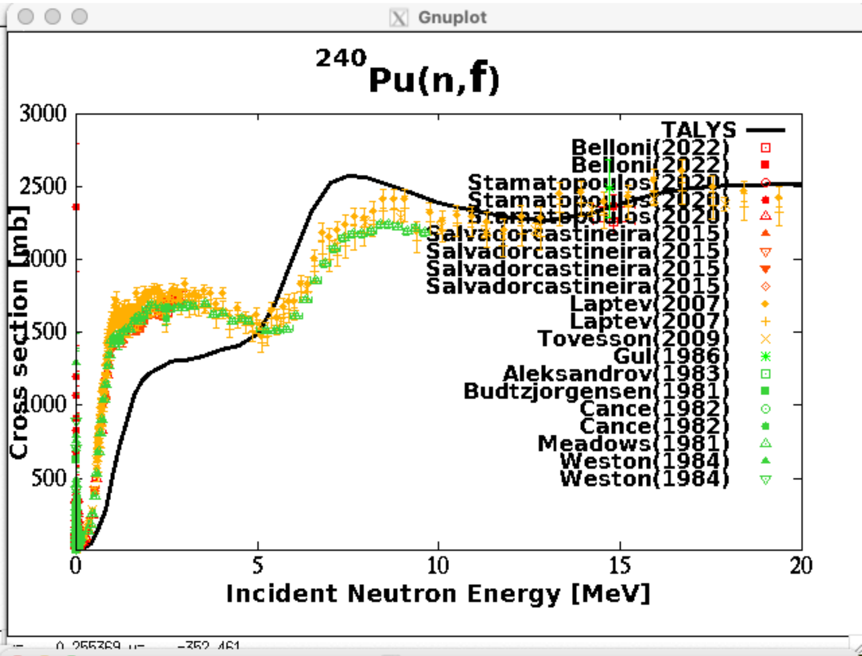
Global calculations for U isotopes: low energies

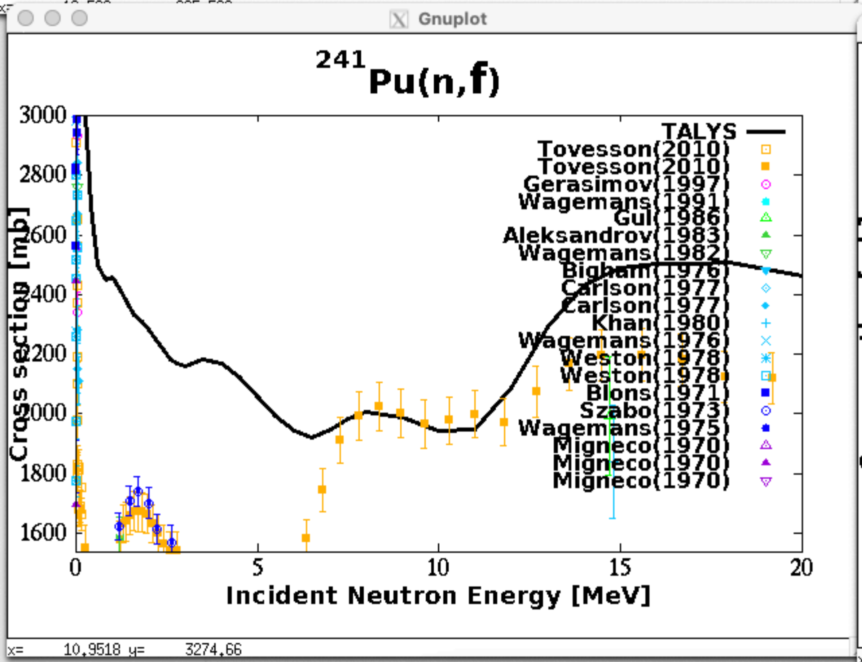


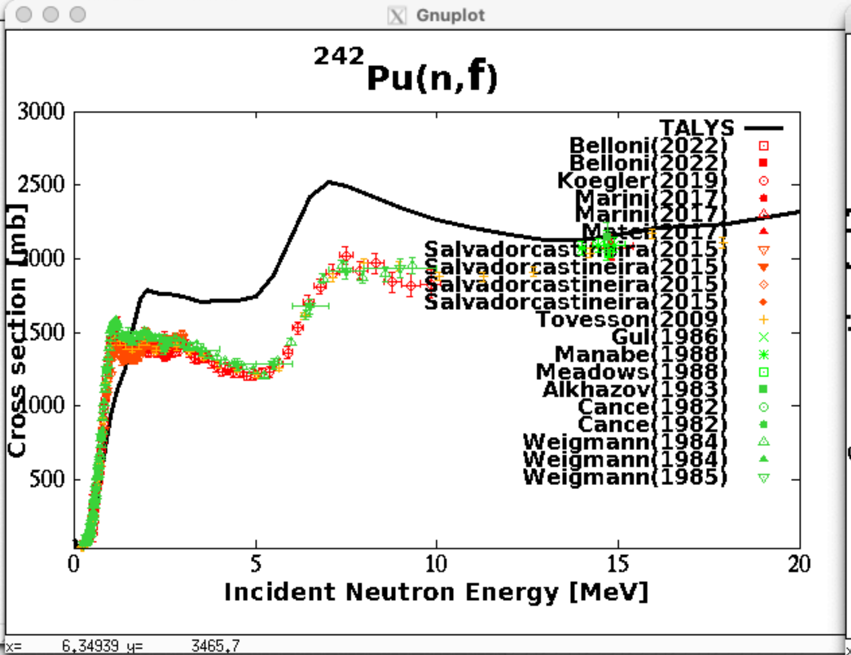
Global calculations for Pu isotopes

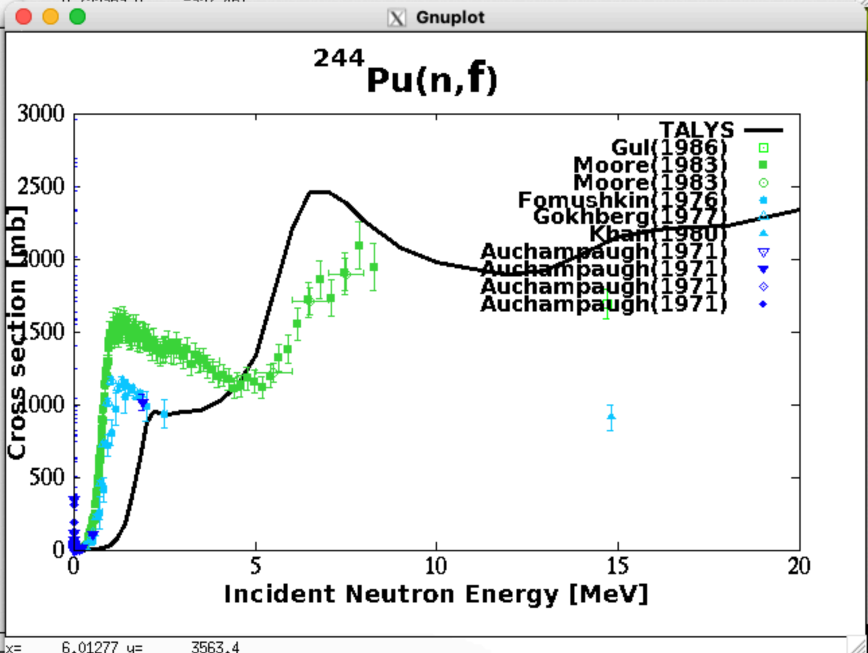




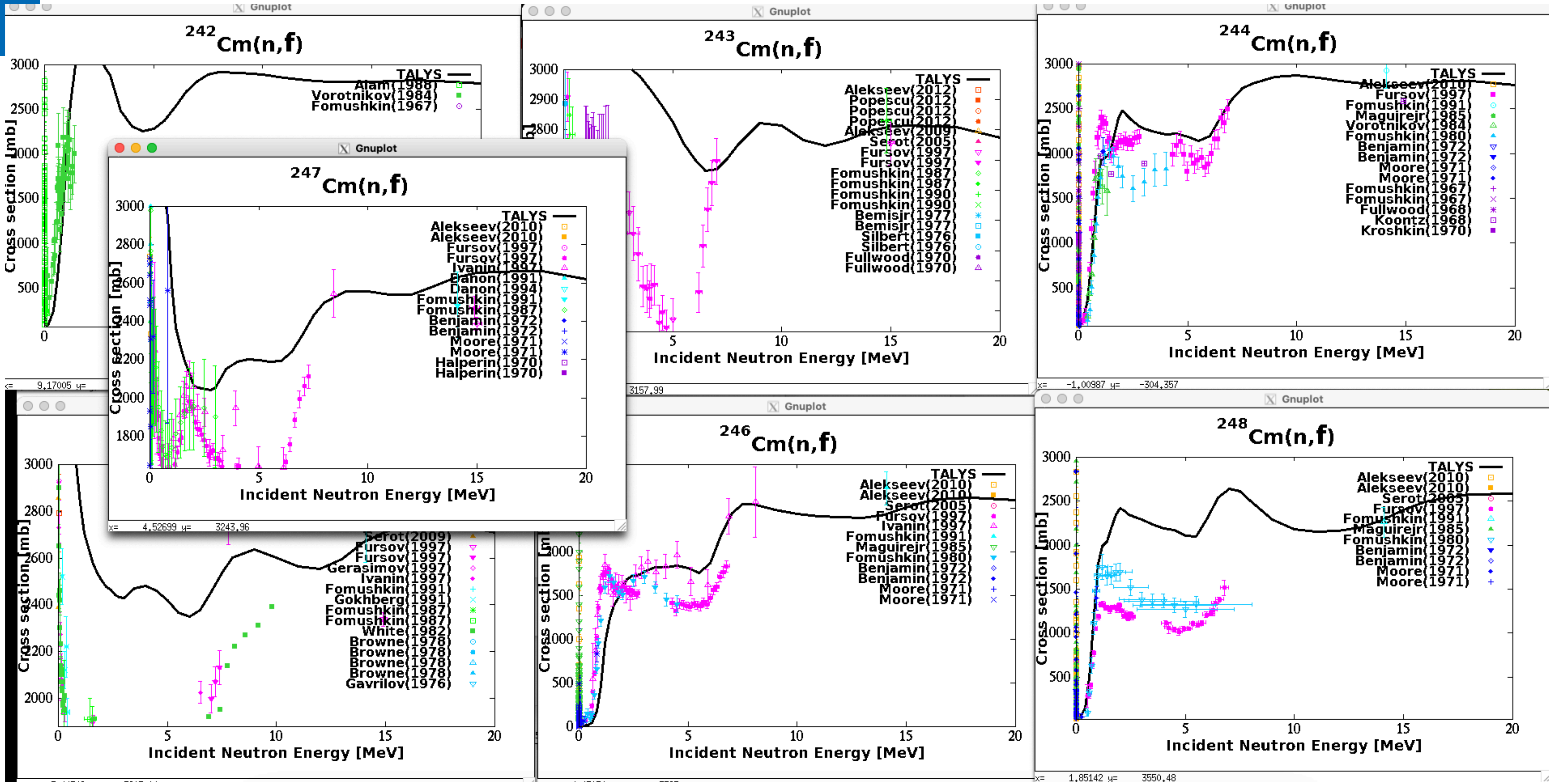








Global calculations for Cm isotopes



Optimised calculations for first chance fission

n + U235

```
vfiscor       92 236    1.07563
rmiufiscor    92 236    1.00377
ptable        92 236    1.00221 1
ptable        92 236 -6.54958E-01 2
ctable        92 236    0.70130 1
ctable        92 236 -2.10926E-01 2
```

n + U236

```
vfiscor       92 237    0.97949
rmiufiscor    92 237    2.69609
ptable        92 237  3.31548E-02 1
ptable        92 237 -9.66362E-02 2
ctable        92 237 -6.99929E-01 1
ctable        92 237    0.52201 2
```

n + U237

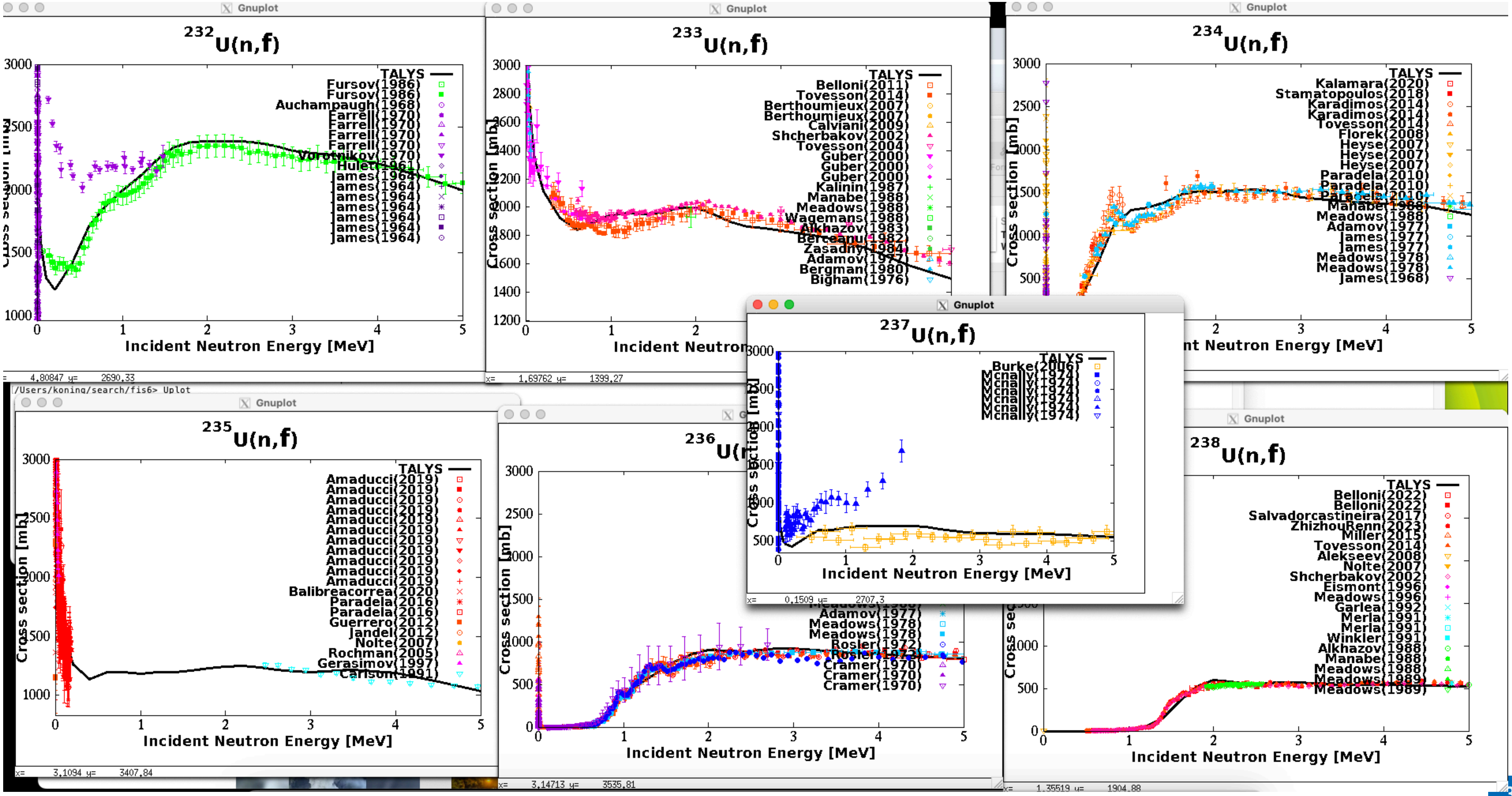
```
vfiscor       92 238    1.11323
rmiufiscor    92 238    1.00406
ptable        92 238 -3.99120E-01 1
ptable        92 238 -2.48911E-01 2
ctable        92 238 -7.73517E-01 1
ctable        92 238    0.72054 2
```

n + U238

```
vfiscor       92 239    0.97616
rmiufiscor    92 239    4.09798
ptable        92 239    0.31892 1
ptable        92 239 -1.64754E+00 2
ctable        92 239 -7.88795E-01 1
ctable        92 239 -3.89683E-03 2
```

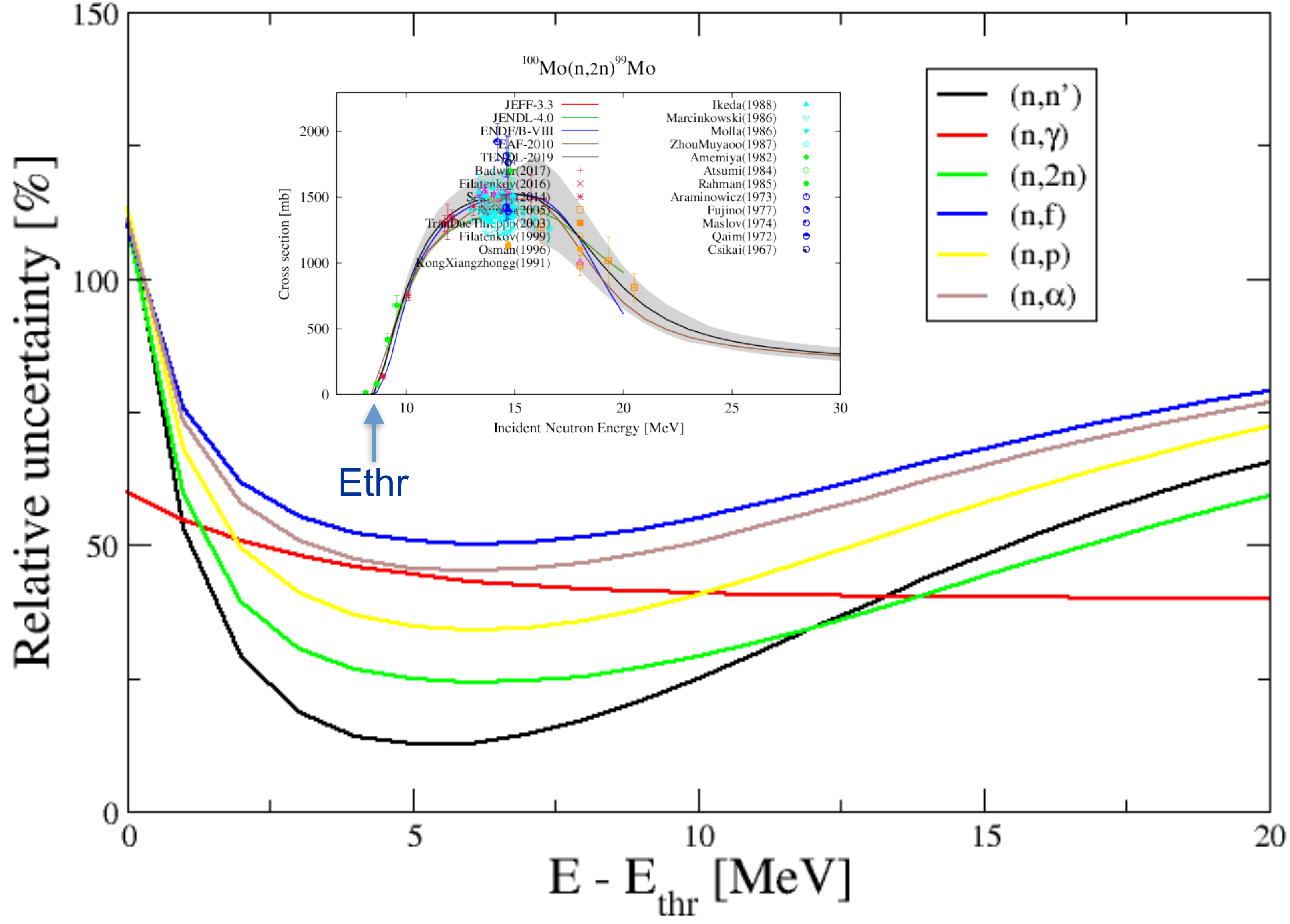
Use these parameters separately for first-chance fission calculation.
Also with ‘ngfit y’
Keep ground-state level density parameters untouched.

Optimised calculations for first chance fission: U isotopes



Global predictive power of TALYS

Based on all EXFOR cross sections, A-independent



Summary, observations, questions

- TALYS seems to be reaching convergence (unfortunately) for global predictive power:
  - (n,γ) in fast range: ~40%
  - (n,f) in fast range: 50-80%
  - (n,n’): ~20%, (n,2n): ~30%, (n,p): ~40%, (n,α): ~50%
  - Above numbers hold for global calculations versus measured reaction channels, i.e. the 200-300 most ‘important’ nuclides
  - Above numbers after serious exforcism.
  - We assume this to be applicable for unmeasured nuclides close to stability
  - Estimate for shorter lived nuclides underway (see Goriely)
- Significant improvement of **descrip**tive power with relative small number of parameters (—> TENDL, JEFF), i.e. smaller deviations than the global numbers above.
- Consolidated, readable, computer accessible (and ideally: evaluated) experimental nuclear reaction database essential for assessment of quality of nuclear models.

Thank you for your attention!