AZURE2 Development Status and ^{7}Be Compound Evaluation

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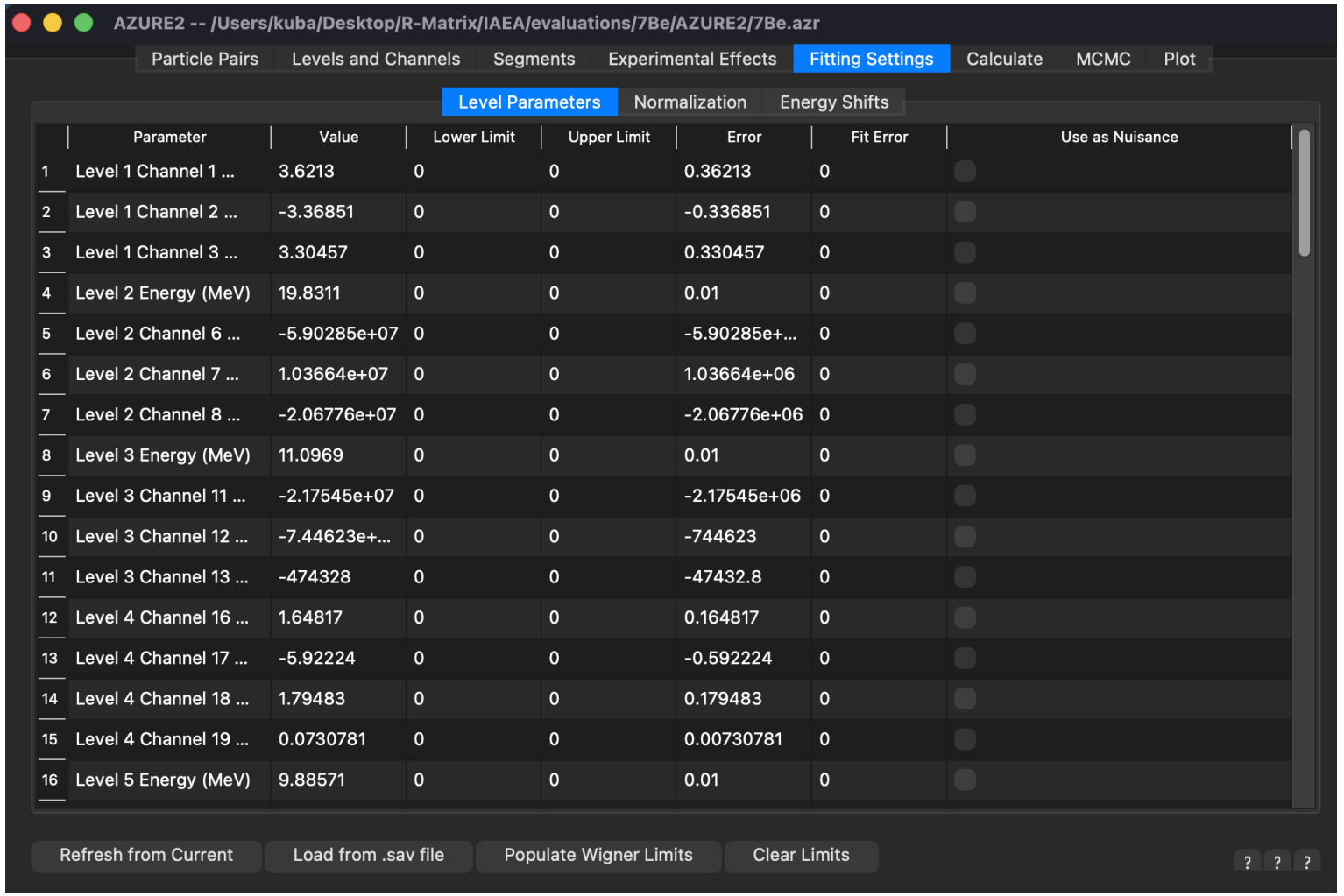
20/11/2025

AZURE2
Development

AZURE2 Improvements

1. Fitting Tab
2. **Wigner Limit** Calculation
3. **Energy Shifts** Addition
4. Reaction Channel **Summing** / **Ratioing**
5. **Coulomb Wavefunction**
6. **Infinite Target Yields**
7. (Experimental) Alternative Minimizers
8. (Experimental) **Native** MCMC Sampler
9. (Experimental) Hybrid Potential Model

AZURE2: Fitting Tab



	Parameter	Value	Lower Limit	Upper Limit	Error	Fit Error	Use as Nuisance
1	Level 1 Channel 1 ...	3.6213	0	0	0.36213	0	
2	Level 1 Channel 2 ...	-3.36851	0	0	-0.336851	0	
3	Level 1 Channel 3 ...	3.30457	0	0	0.330457	0	
4	Level 2 Energy (MeV)	19.8311	0	0	0.01	0	
5	Level 2 Channel 6 ...	-5.90285e+07	0	0	-5.90285e+...	0	
6	Level 2 Channel 7 ...	1.03664e+07	0	0	1.03664e+06	0	
7	Level 2 Channel 8 ...	-2.06776e+07	0	0	-2.06776e+06	0	
8	Level 3 Energy (MeV)	11.0969	0	0	0.01	0	
9	Level 3 Channel 11 ...	-2.17545e+07	0	0	-2.17545e+06	0	
10	Level 3 Channel 12 ...	-7.44623e+...	0	0	-744623	0	
11	Level 3 Channel 13 ...	-474328	0	0	-47432.8	0	
12	Level 4 Channel 16 ...	1.64817	0	0	0.164817	0	
13	Level 4 Channel 17 ...	-5.92224	0	0	-0.592224	0	
14	Level 4 Channel 18 ...	1.79483	0	0	0.179483	0	
15	Level 4 Channel 19 ...	0.0730781	0	0	0.00730781	0	
16	Level 5 Energy (MeV)	9.88571	0	0	0.01	0	

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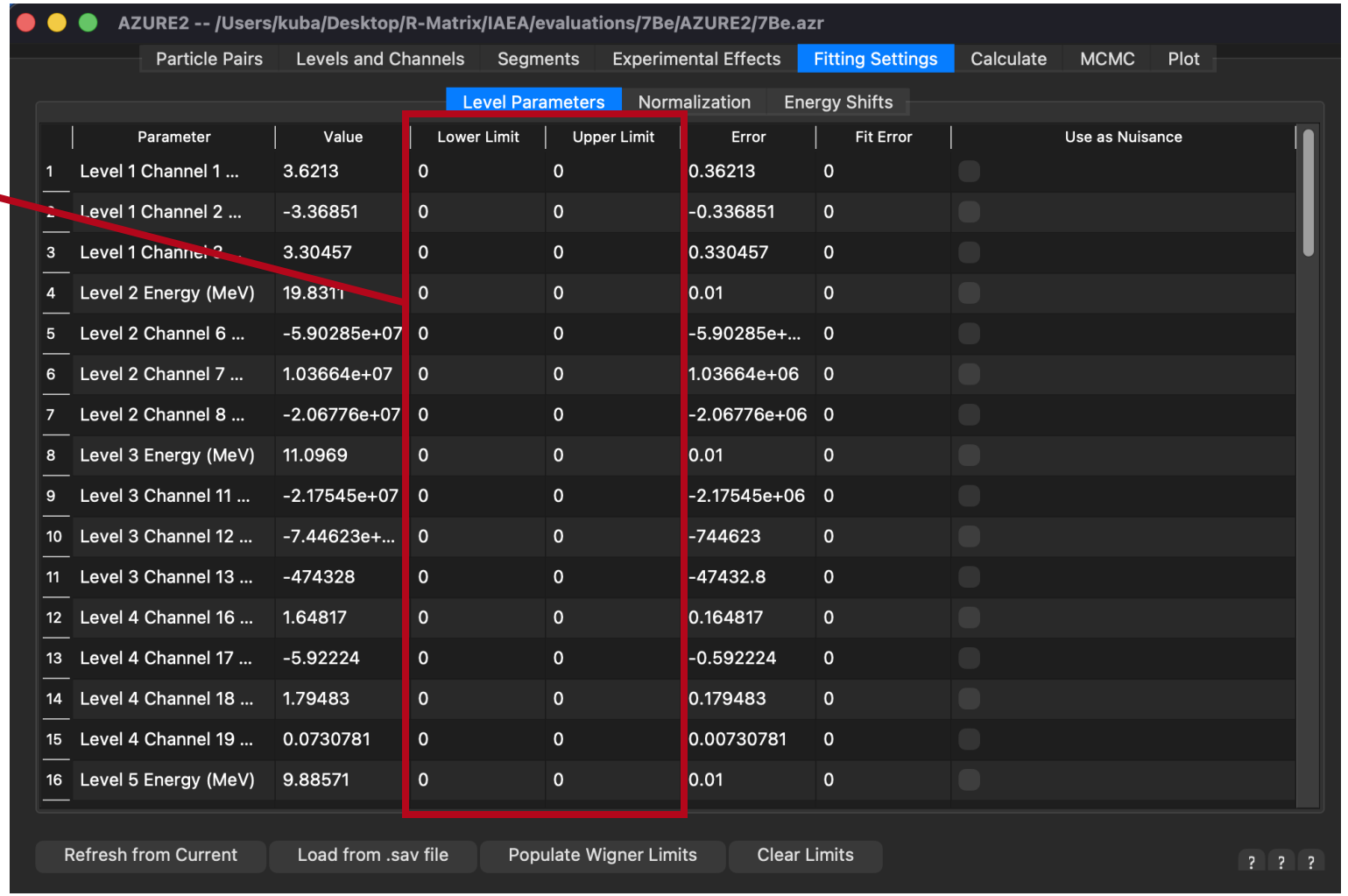
- Possibility of adding **lower** and **upper limits** for each parameter



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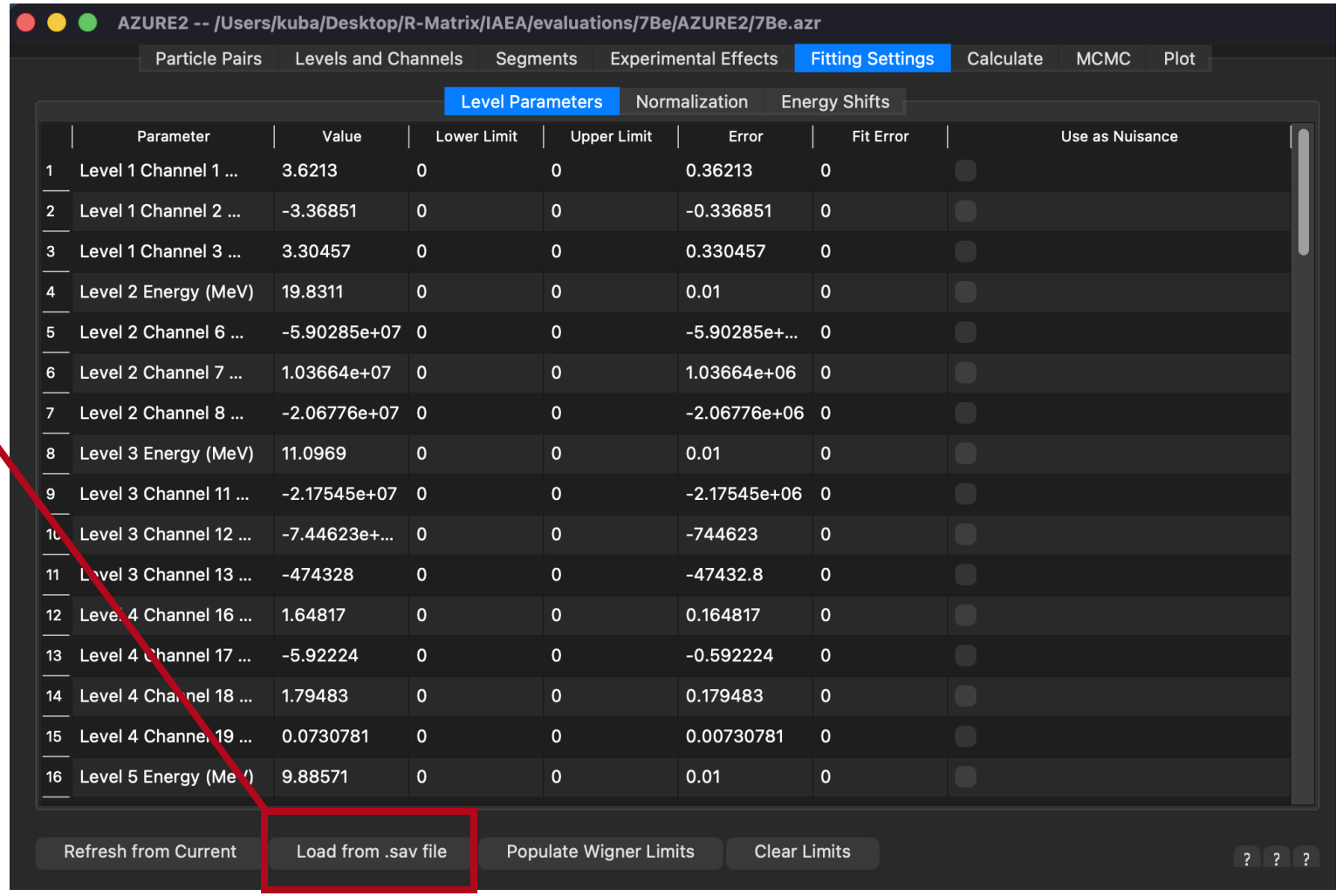

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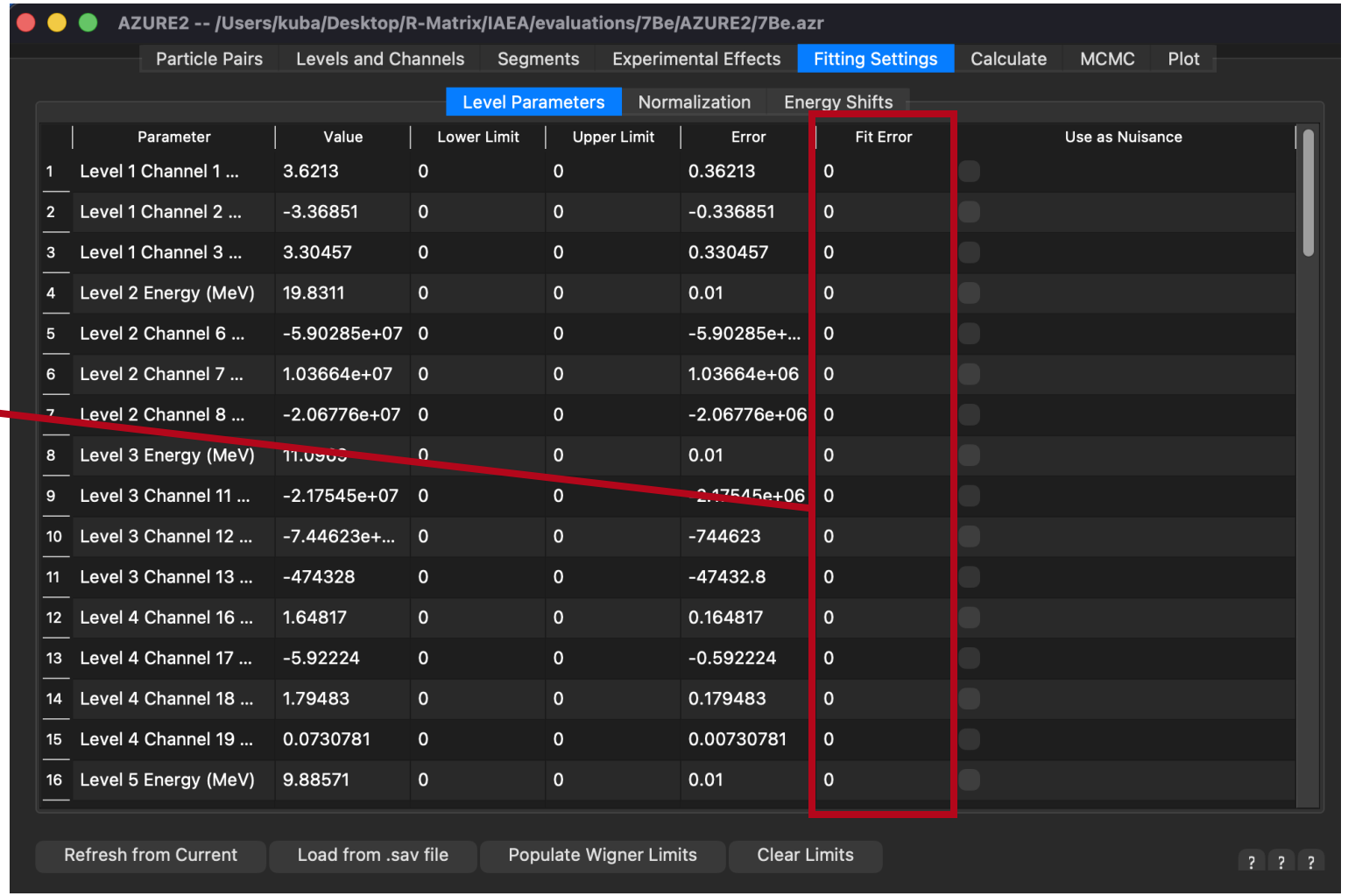

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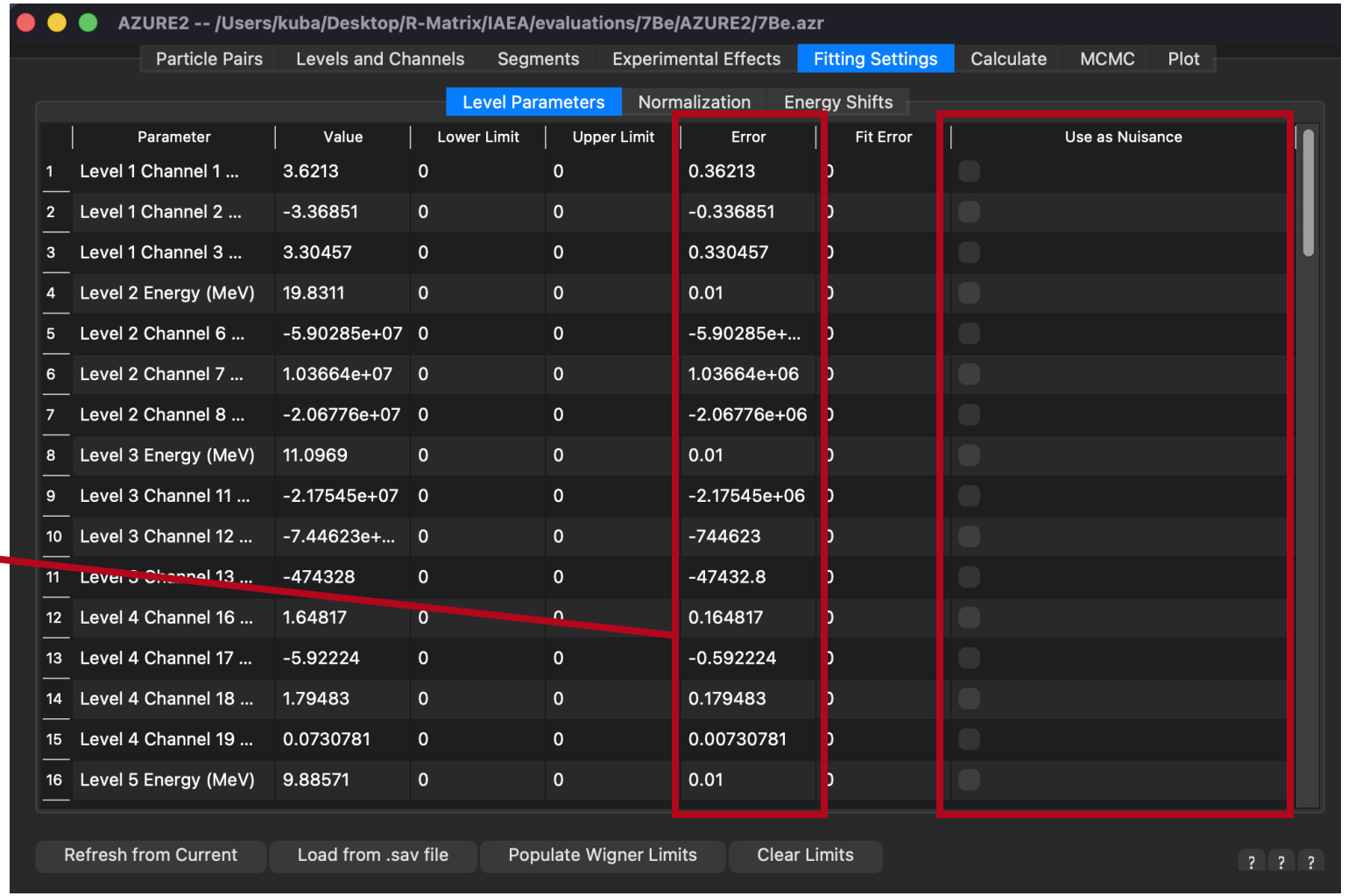
- **Update** of the AZURE2 file with the best-fit parameters
- **Fit error** visualization
- Possibility of using a parameter as a **nuisance parameter**

$$\chi^2 = \left(\frac{p - p_{\text{set}}}{p_{\text{err}}} \right)_i^2$$



AZURE2: Wigner Limits

The **Wigner Limits** are calculated as:

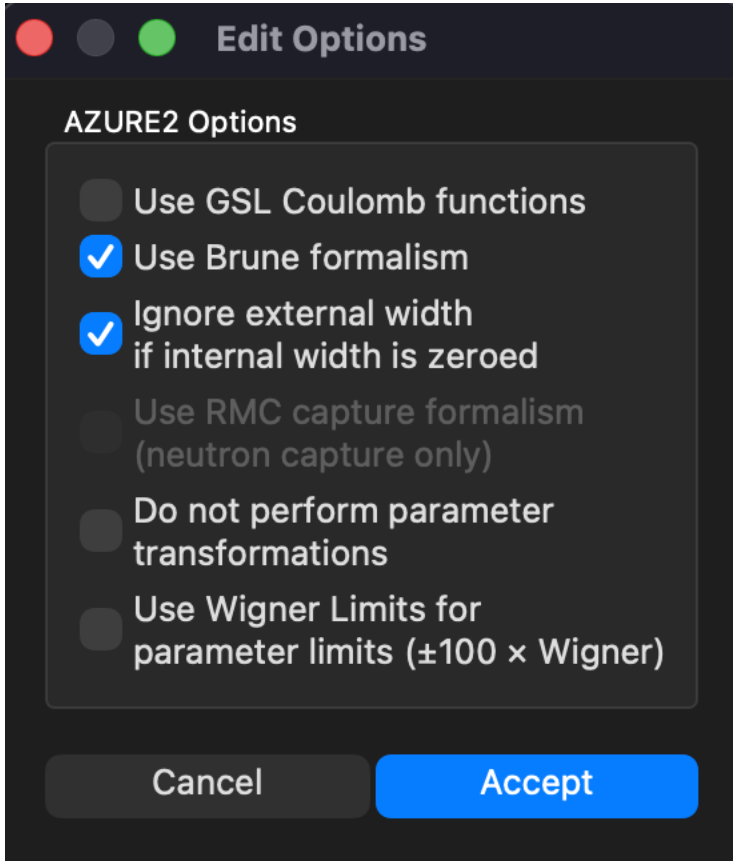
$$\gamma_W^2 = \frac{3\hbar^2}{2\mu a^2}$$

μ : reduced mass

a : channel radius

P. Descouvemont et al. (2010), Rep. Prog. Phys. 73, 036301

AZURE2 –> Configure –> Runtime Options



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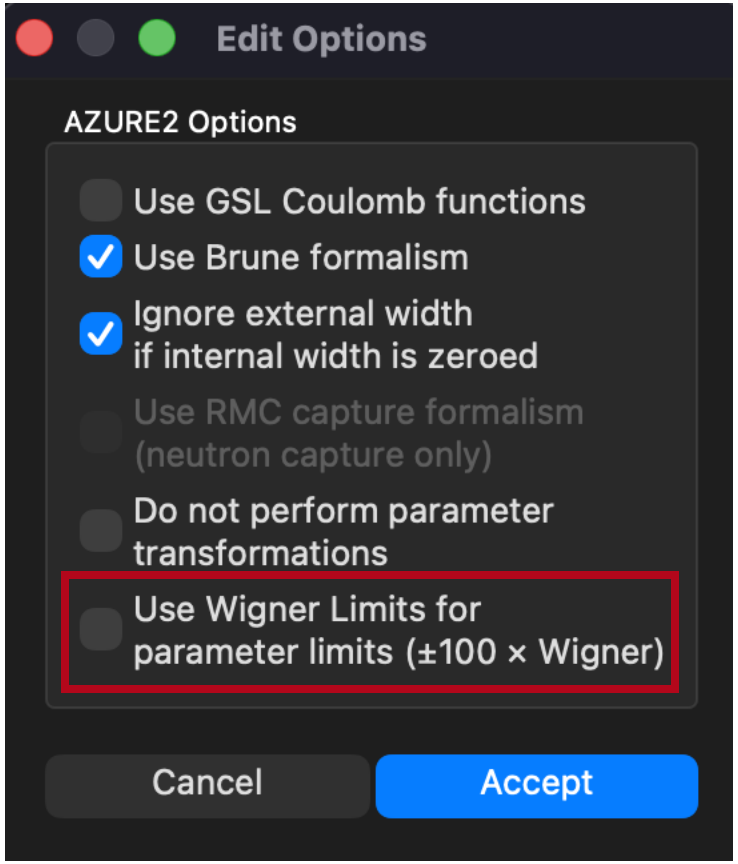

1. The limits are directly applied to the **reduced widths**
2. It is possible to fill the **physical widths** from Fitting Tab

AZURE2: Energy Shifts (1)

One of the major drawbacks in AZURE2 was the **absence of energy uncertainties**

→ **Main Impact**: underestimated uncertainties for the **resonance positions**

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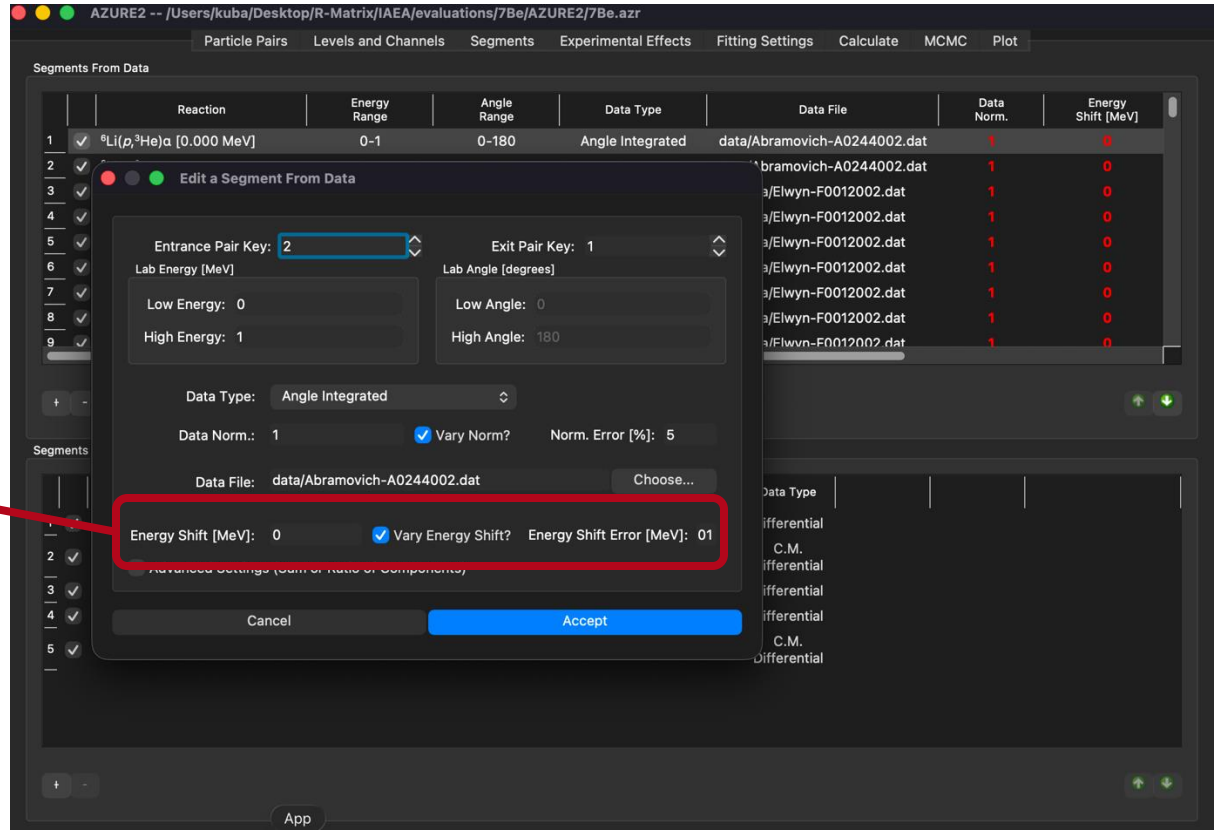
New Energy Shift Term



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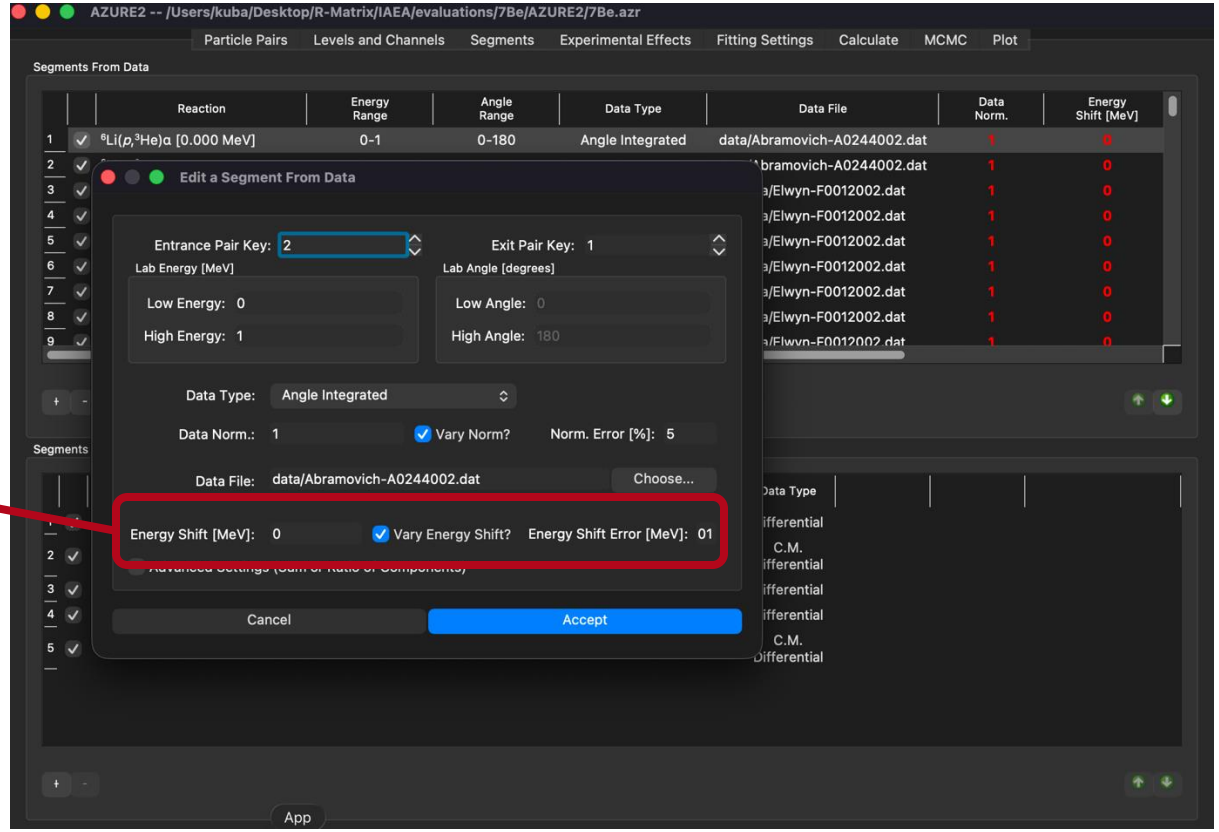
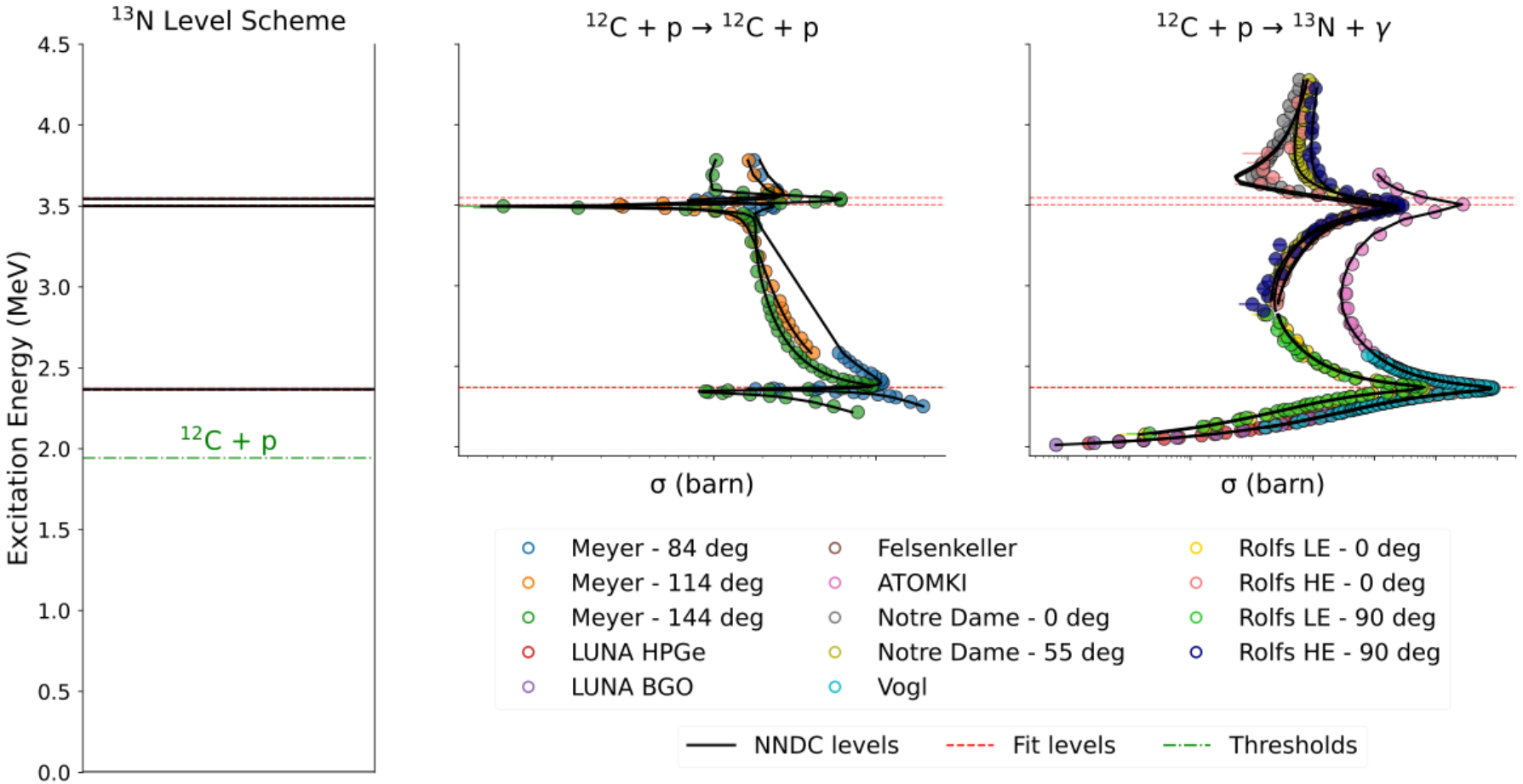


Quite expensive computationally

At each shift change, the code needs to recompute the coulomb wavefunctions…

AZURE2: Energy Shifts (2)

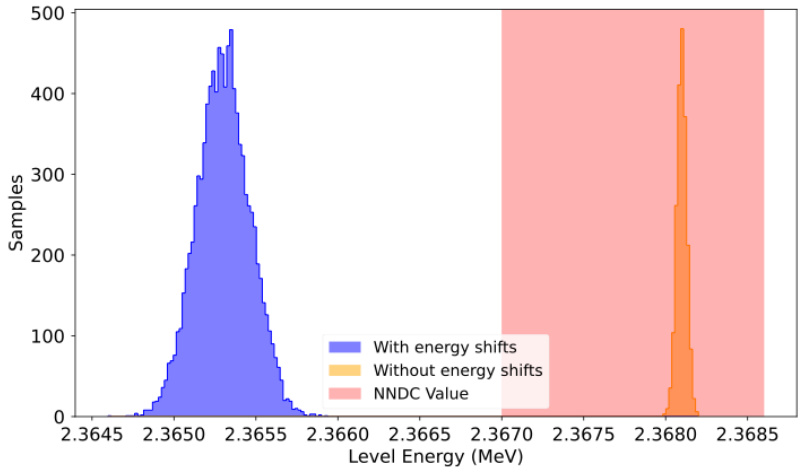


^{12}C(p,γ)^{13}N Benchmark

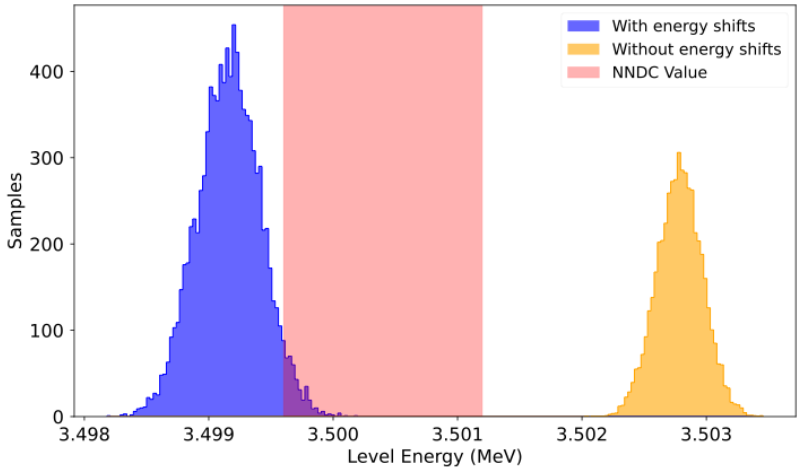
- Frequently used reaction as benchmark
- **Three** different resonances
- **Rolfs** dataset seems to have an **energy shift** w.r.t. to newest data
- **1 keV uncertainty** for the new measurements
- **No uncertainty** for Rolfs and Vogl data

AZURE2: Energy Shifts (3)

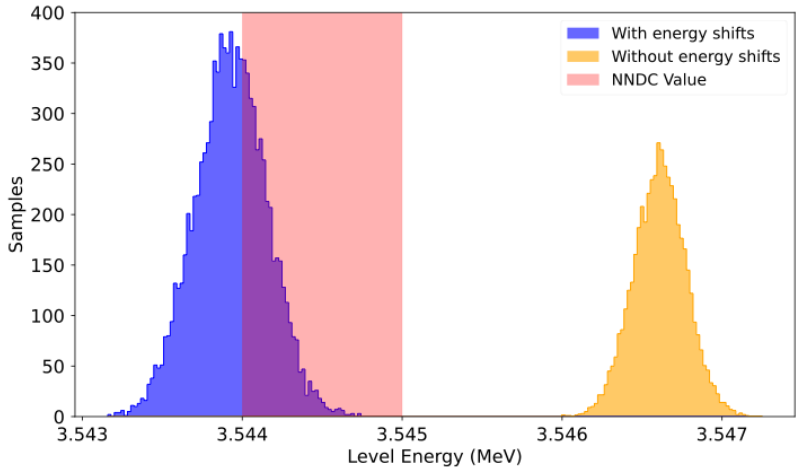
2.365 MeV State



3.503 MeV State



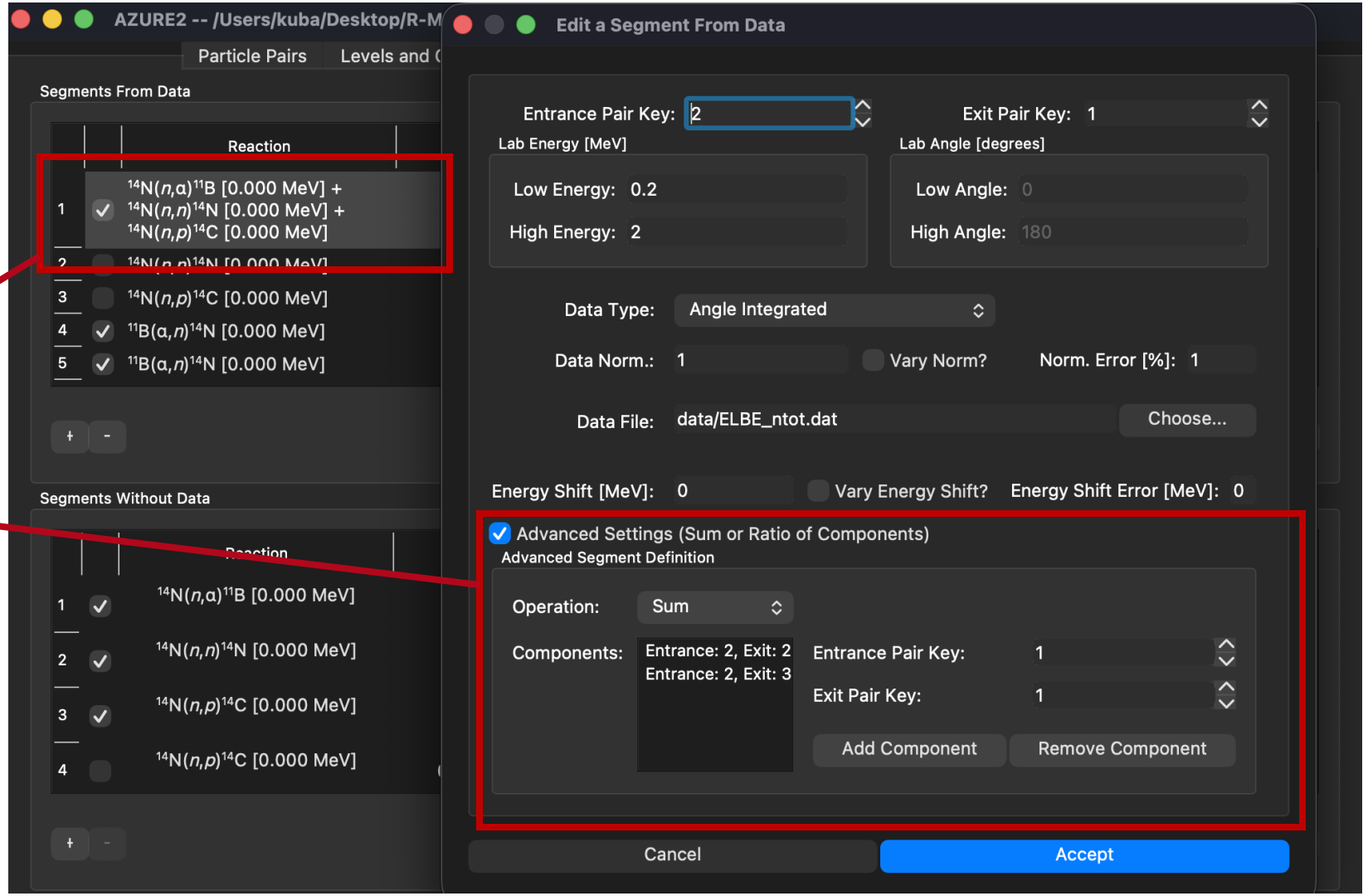
3.545 MeV State



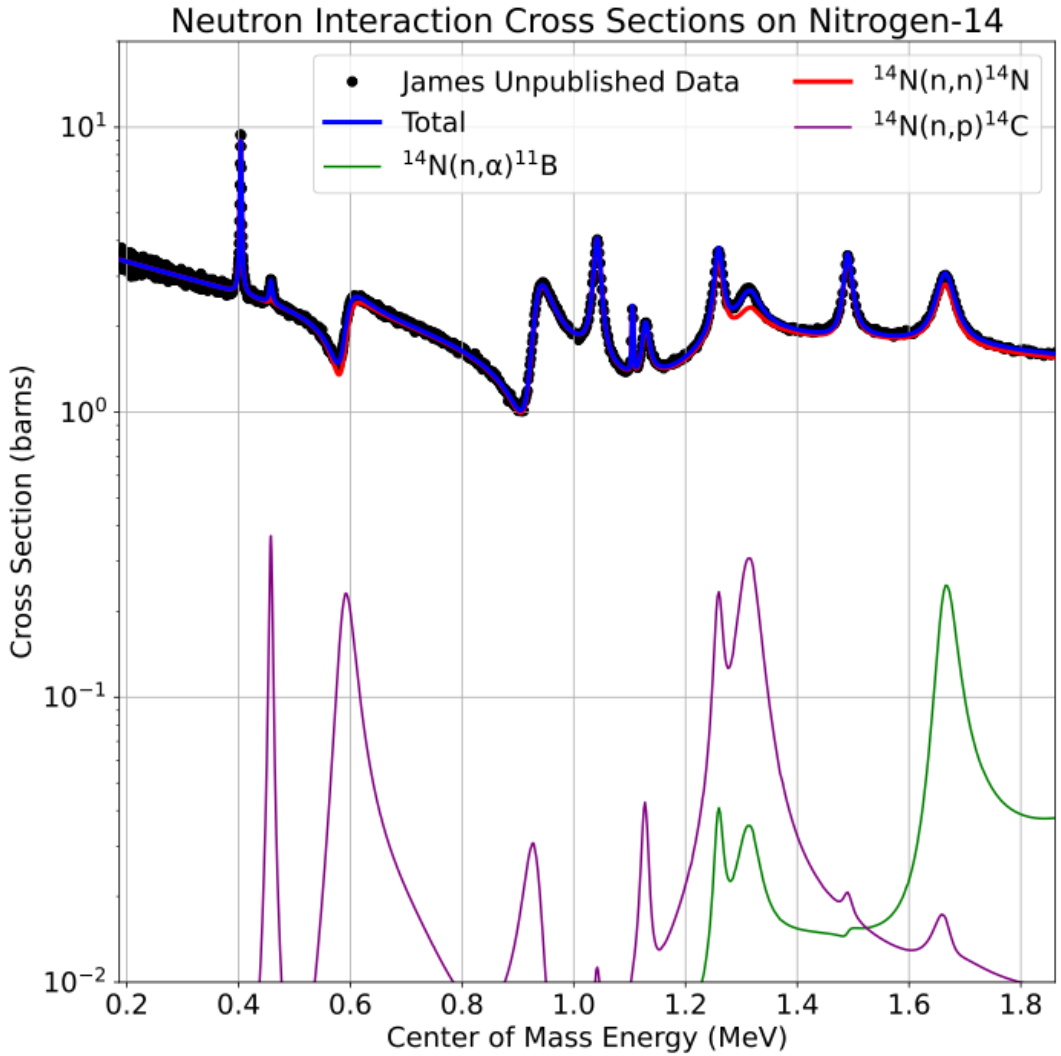
- Without the shifts, the minimizer is **skewed** by the old data
- With the shifts, **broader uncertainty** is found (reliable?)
- The final shift for the Rolfs data is **- 27 ± 1 keV**

AZURE2: Reaction Channel Summing / Ratioing (1)

It's is now possible to define a segment with **multiple input/output channels**



AZURE2: Reaction Channel Summing / Ratioing (2)

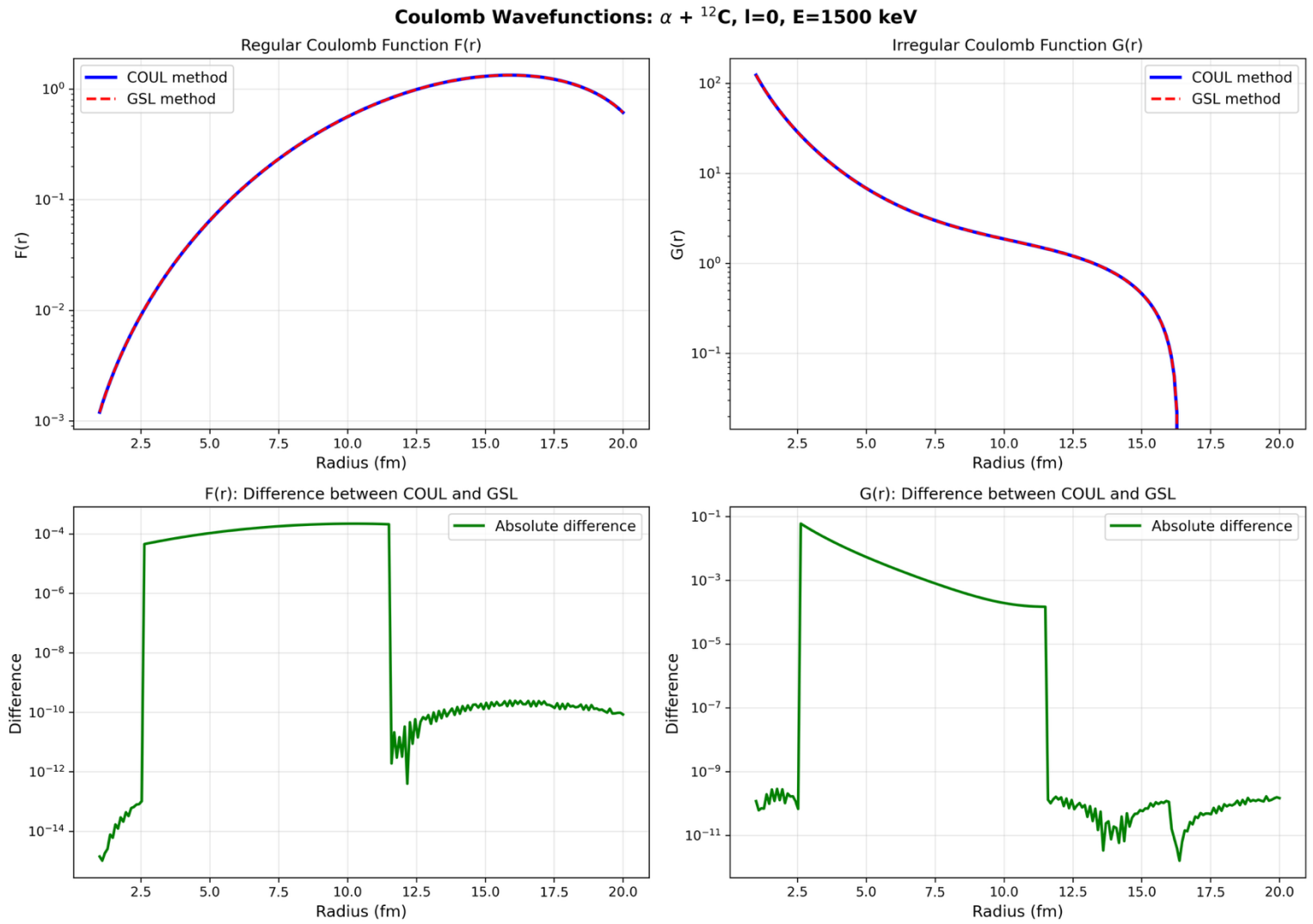


See **James's talk** for more details on the **^{15}N compound** evaluation

AZURE2: Coulomb Wavefunction

Coulomb Wavefunction Improvements

1. A package was created (pycoulomb) to easily test the different CW algorithms



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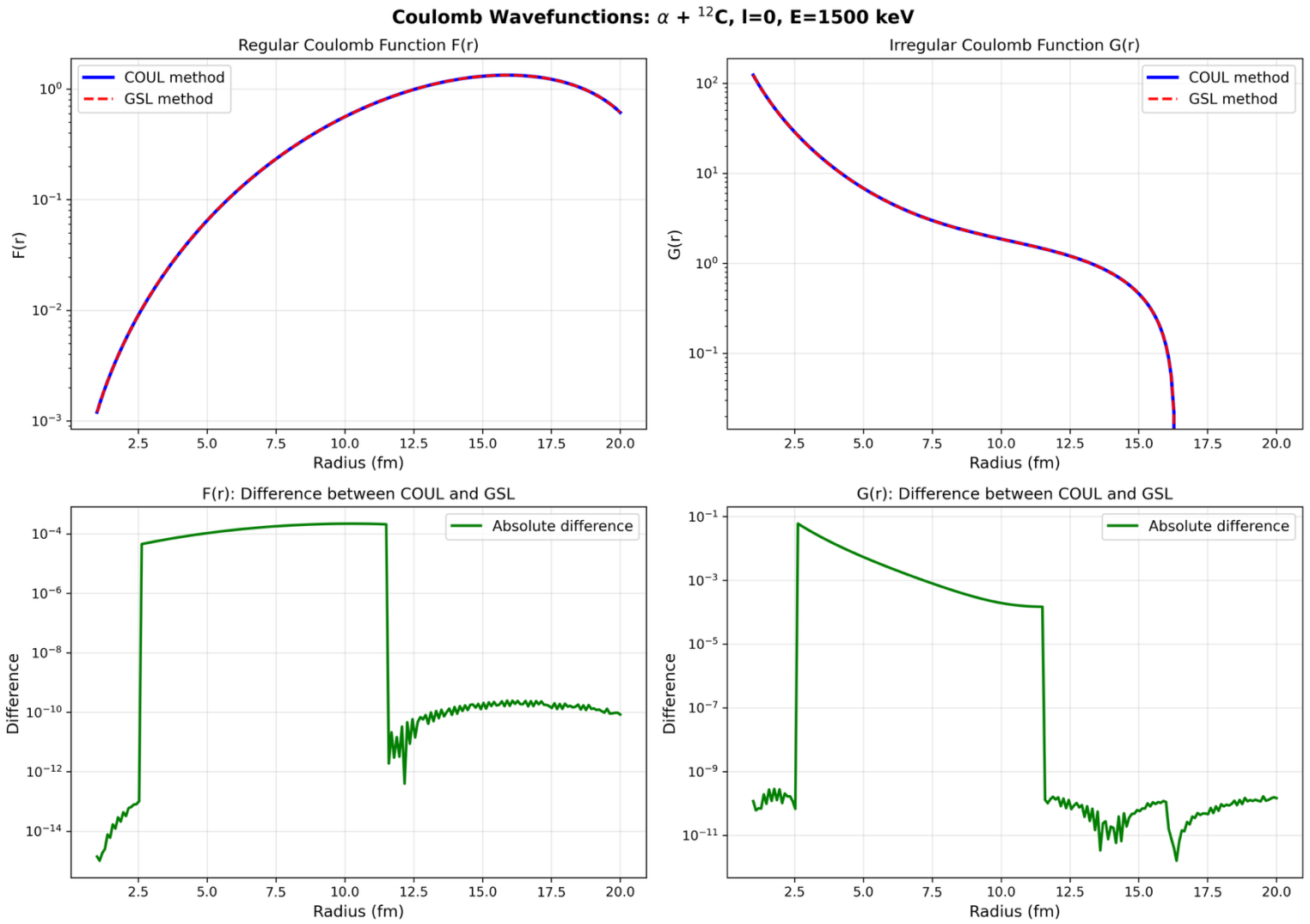

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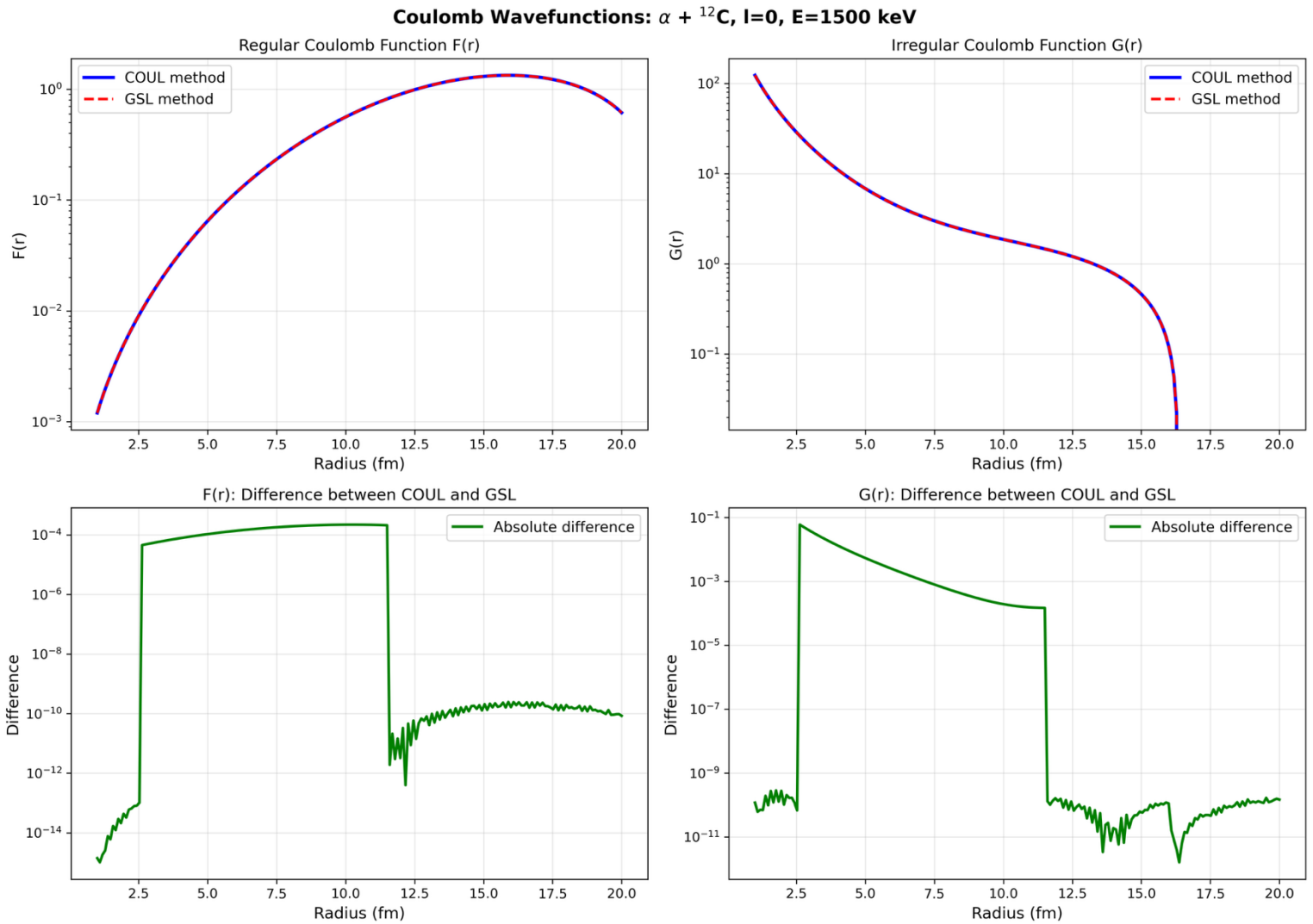
Extrapolations down to 1 eV



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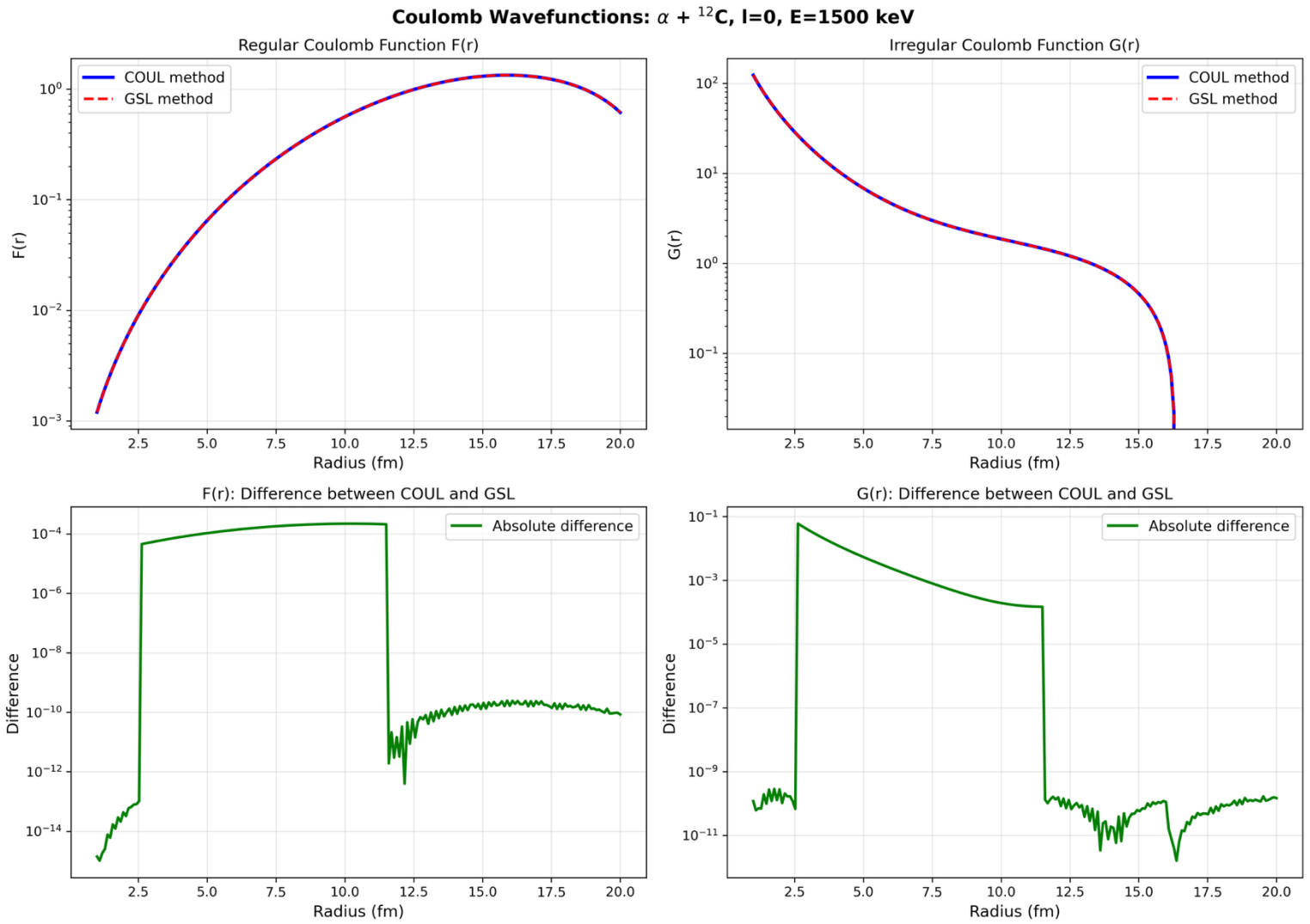
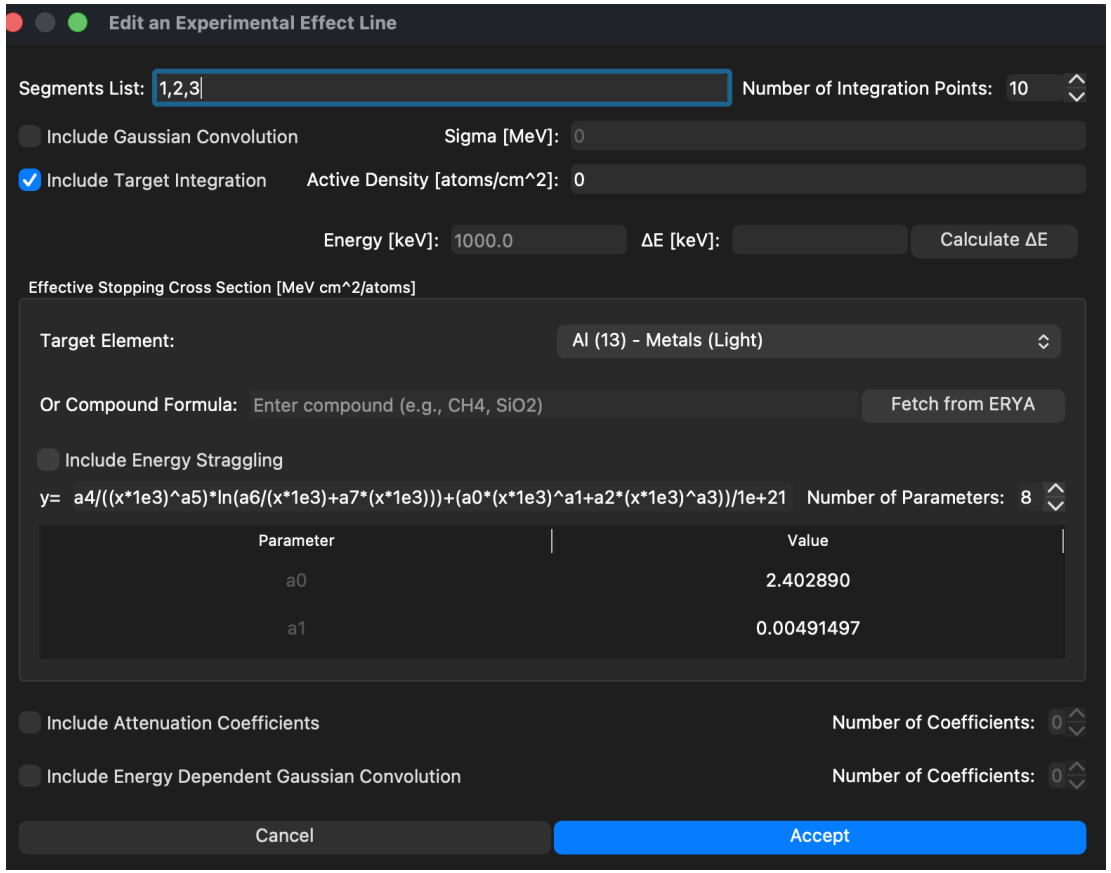
+

x2-5 speed-up from added CW caching system in AZURE2



AZURE2: Infinite Target Yield (1)

AZURE2 is now capable to calculate the **infinitely thick target yield**



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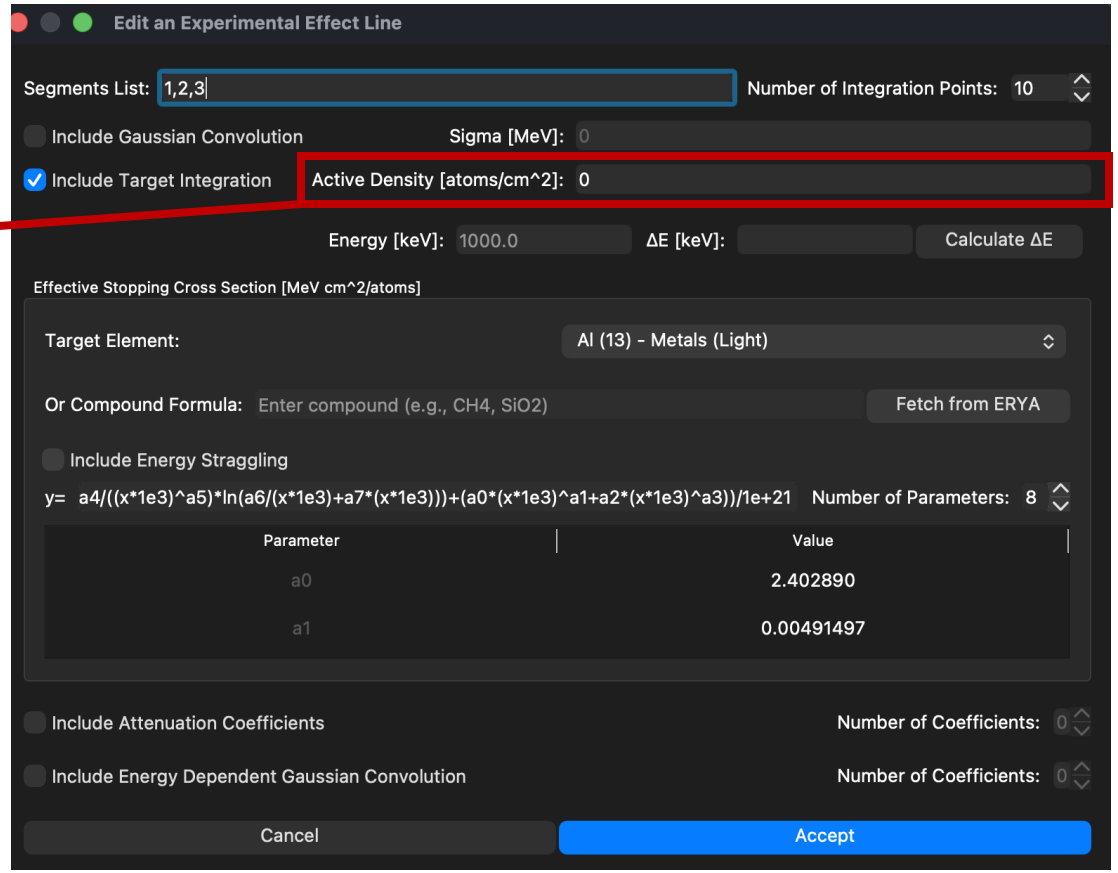
Active Density must be set to **0** to activate the infinite target integration



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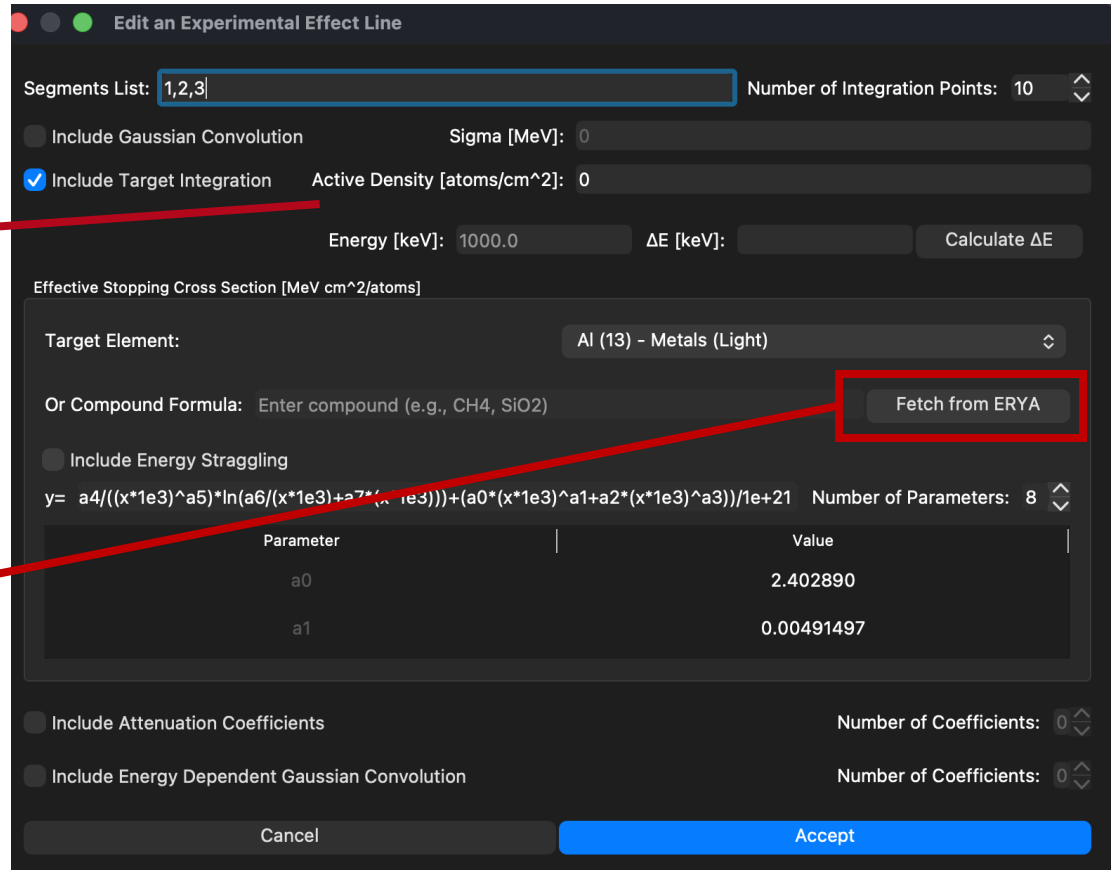
ERYA Stopping Power tables for protons has been introduced for easy retrieval



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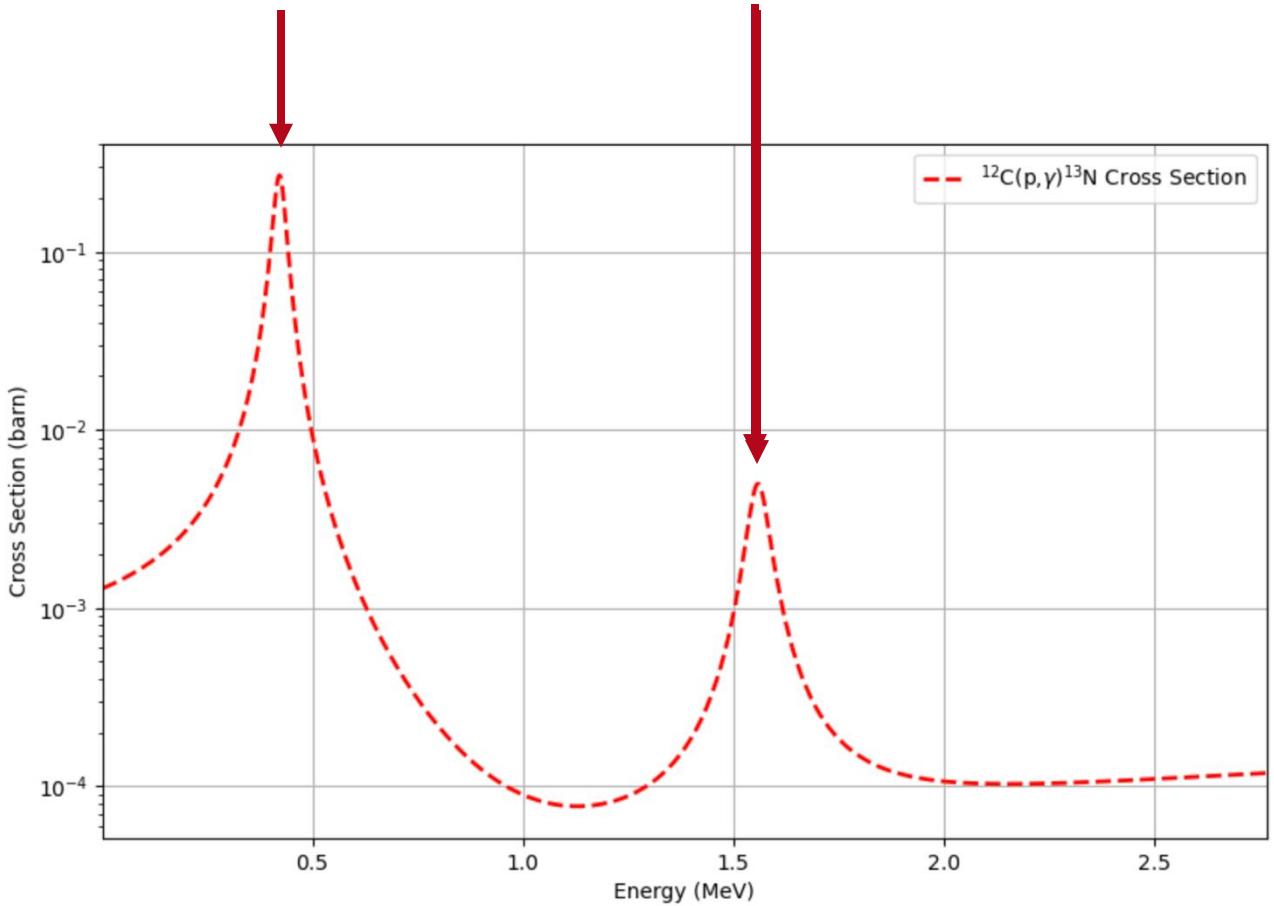
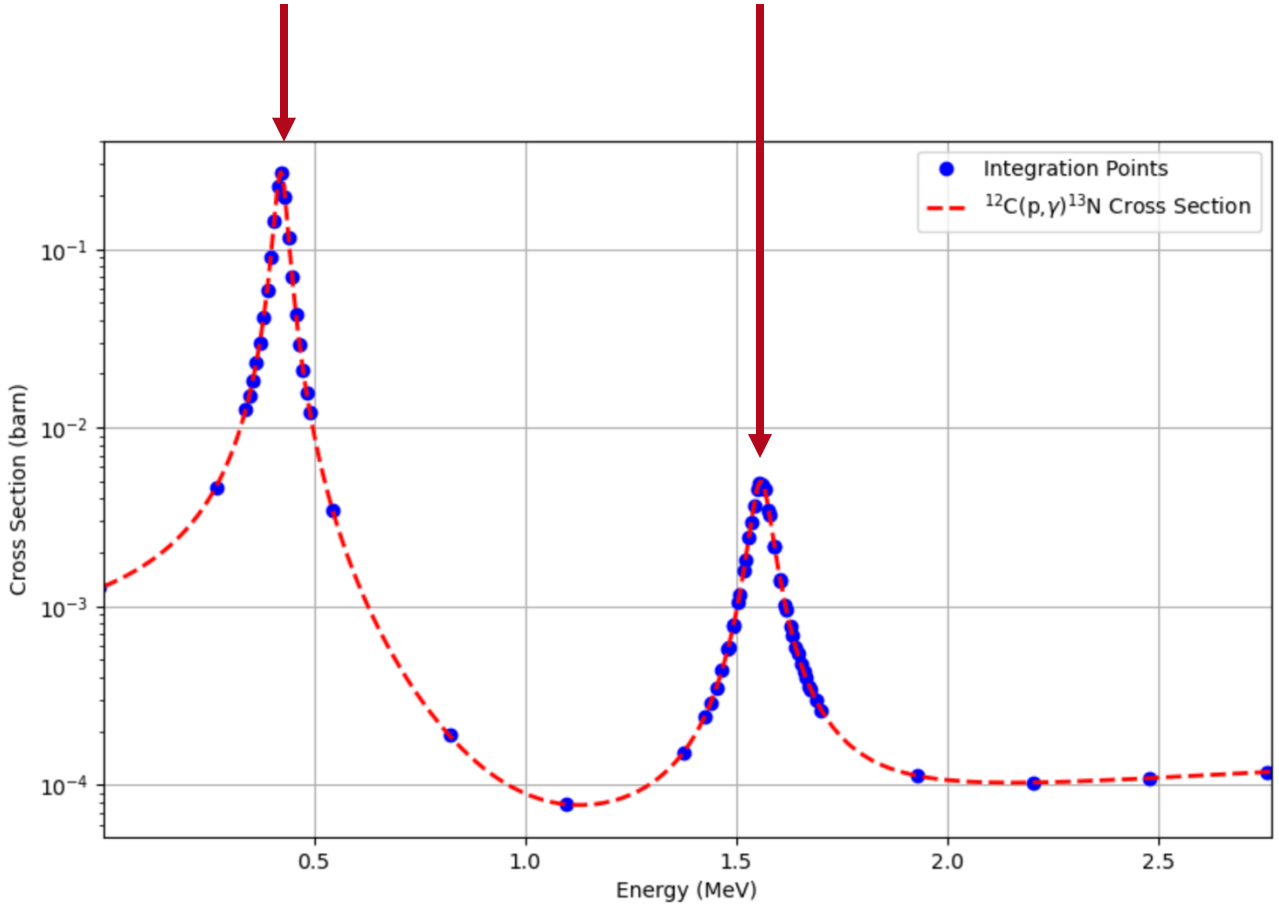


AZURE2: Infinite Target Yield (1)

AZURE2 is now capable to calculate the **infinitely thick target yield**

How It Works

1. Before the calculation, AZURE2 gathers all the resonances
2. Then, basing on each resonance width, it assigns **20 symmetric integration points around each of them**



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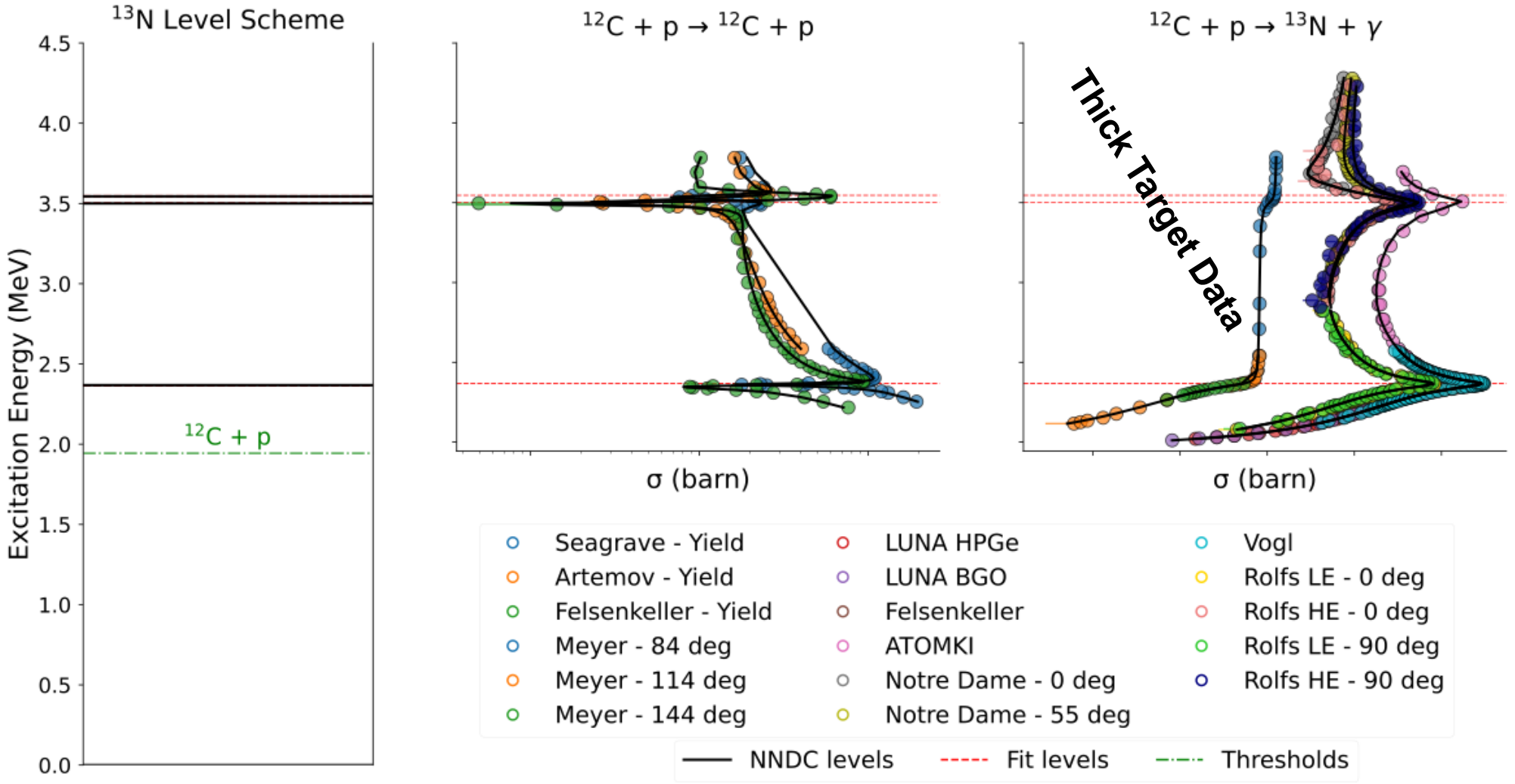
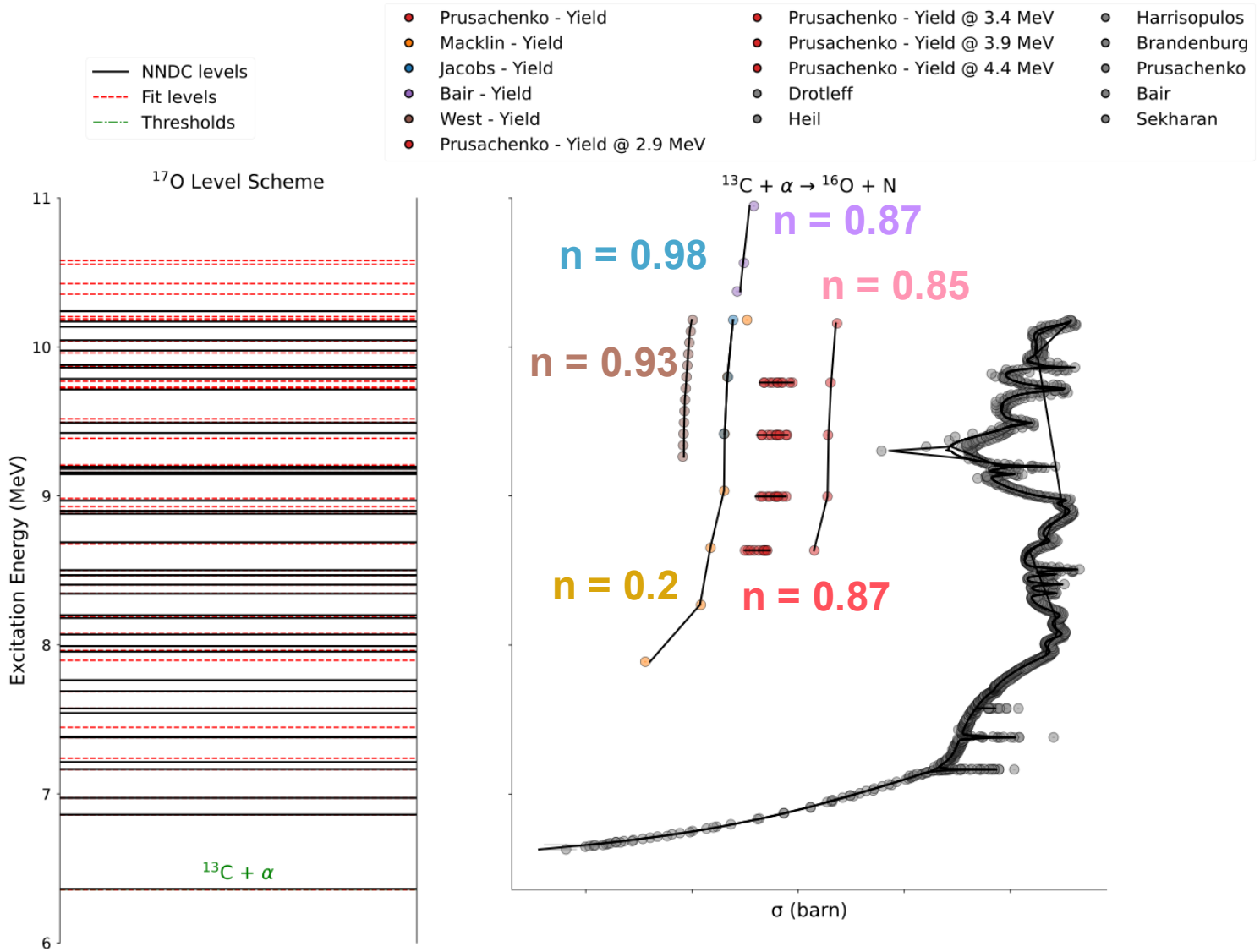


Agrees well with the new data!

AZURE2: Infinite Target Yield (3)

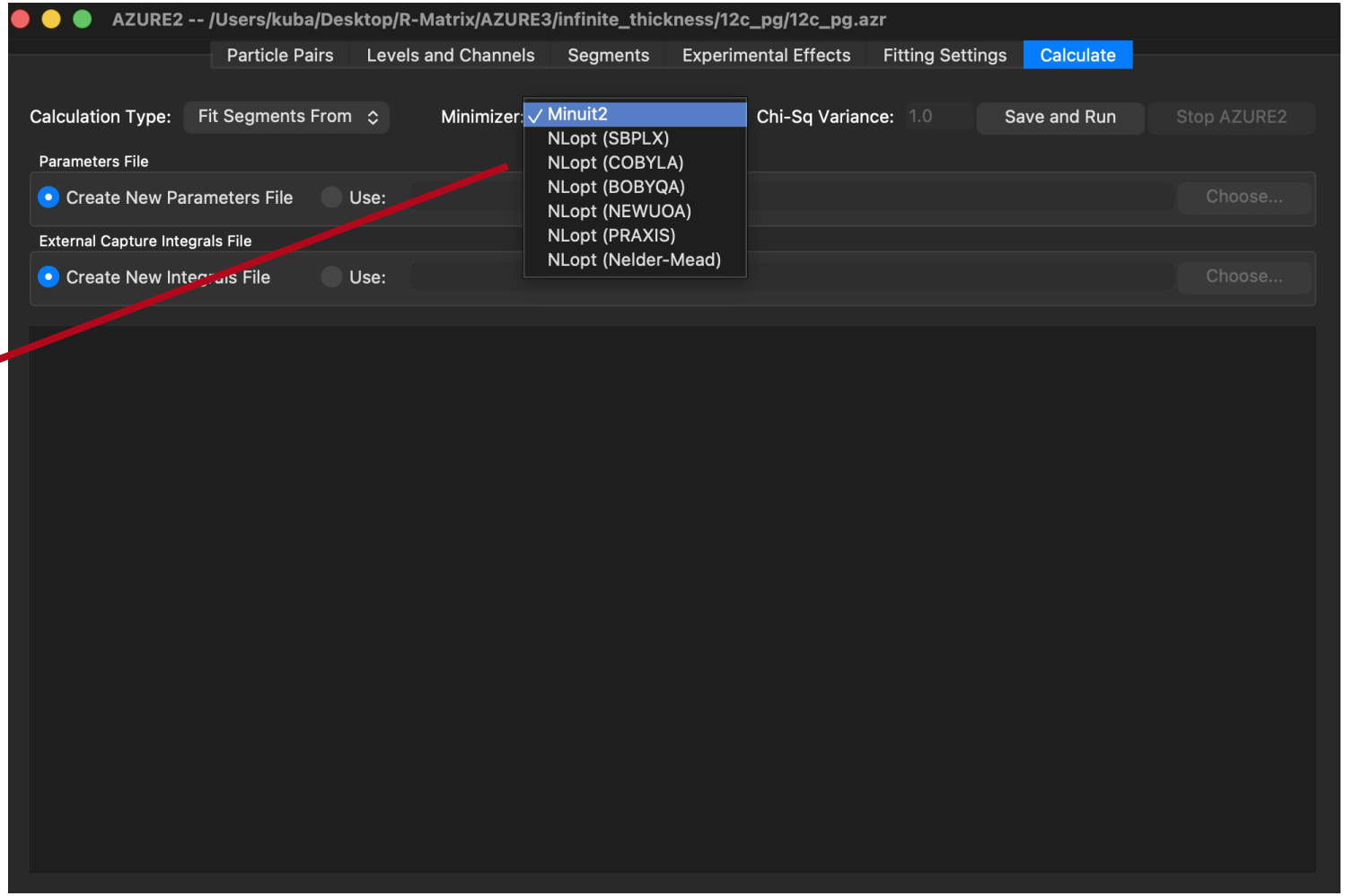


$^{13}C(\alpha,n)^{16}O$

- More complex example
- A lot of thick yield data available in **literature**
- Quite **a good agreement**
- Apart from **Macklin data**

AZURE2: (Experimental) Alternative Minimizers

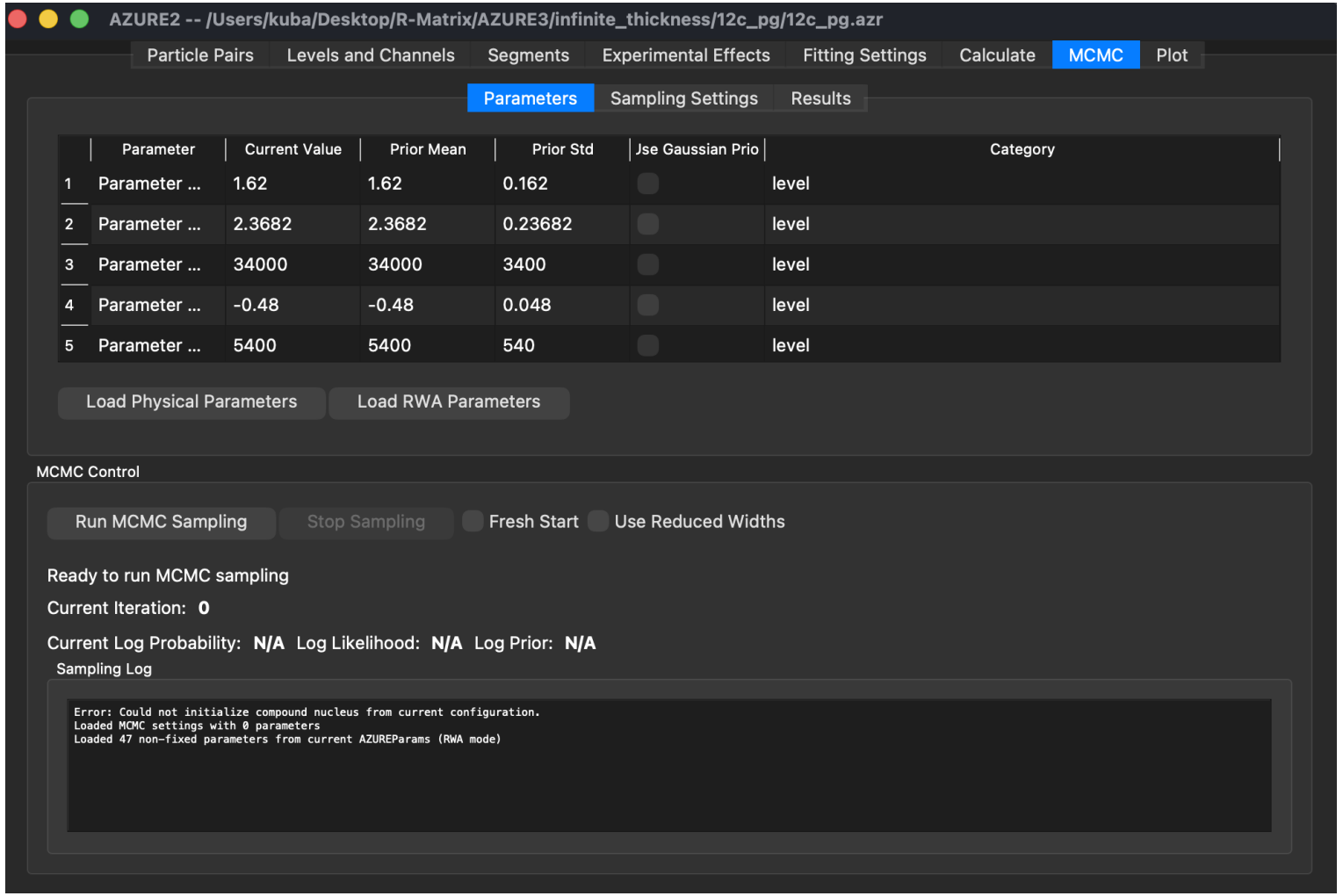
The nlopt library was added with the possibility of using **well-know alternative minimizers**



AZURE2: (Experimental) Native MCMC Sampler

The **numcmc library** (10.5281/zenodo.5496329) was added for a native MCMC sampling

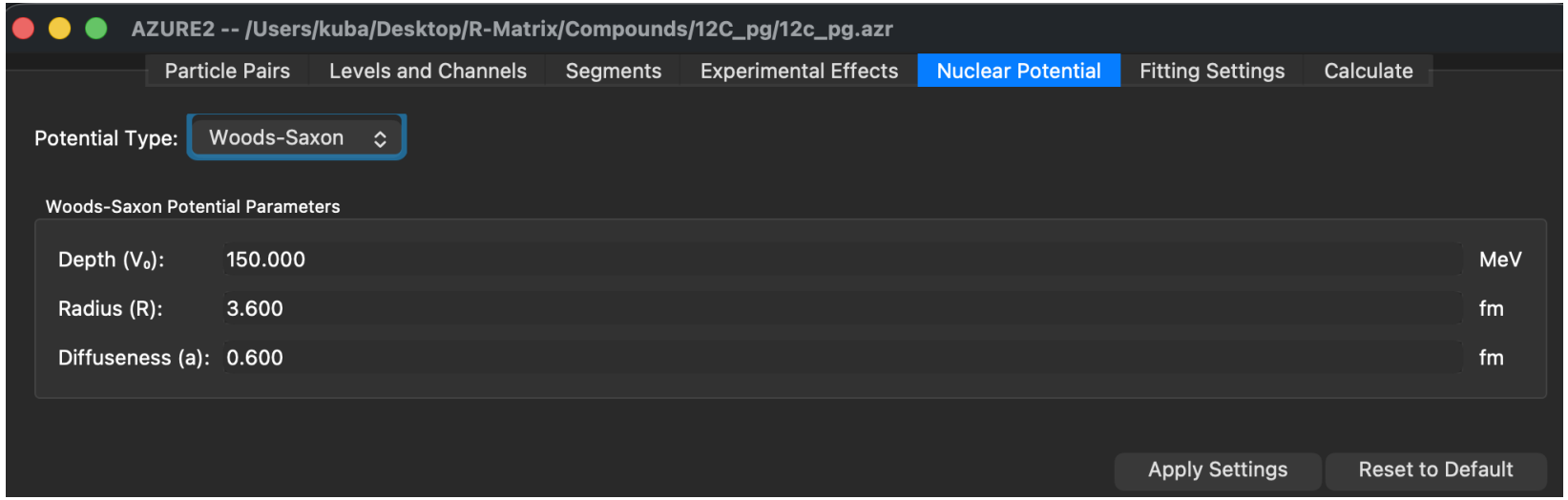
Same MCMC algorithm as the **emcee package** (to be thoroughly tested!)



AZURE2: (Experimental) Hybrid Potential Model

Hybrid Potential Model was implemented in AZURE2

1. Coulomb Wavefunction is calculated at **r = 15 fm** with COUL algorithm
2. Then the wavefunction is obtained at the desired radius by using the **Numerov method**
3. During the integration, a Woods-Saxon potential Is assumed with V_0, a_s and r_s



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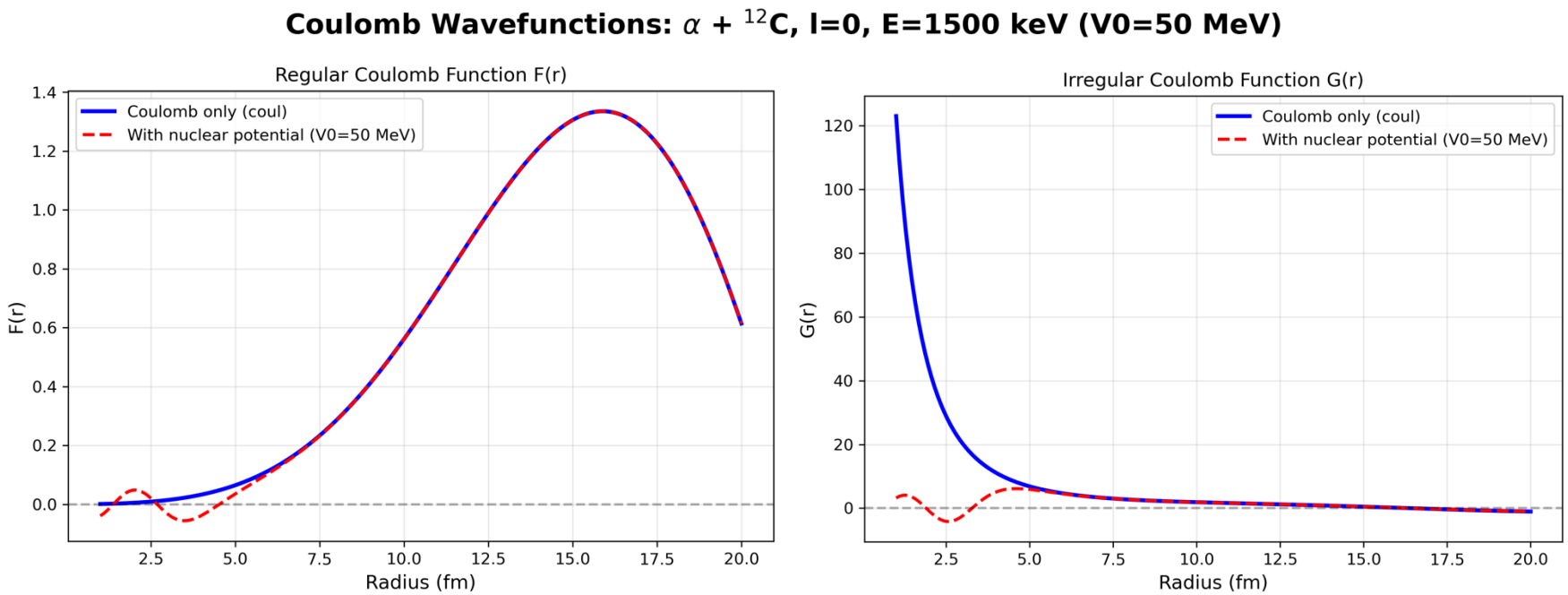
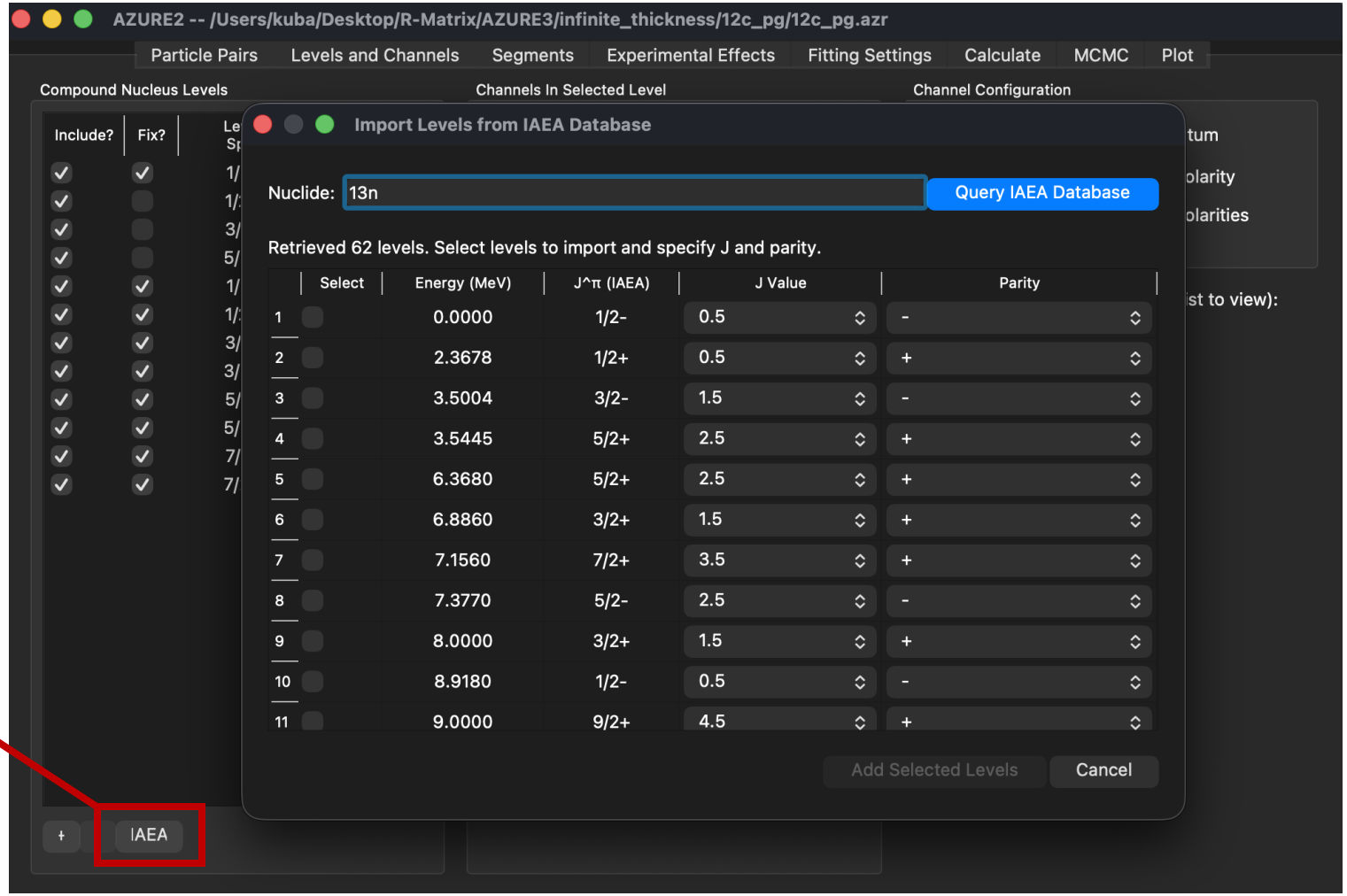
- Already implemented in [pycoulomb]
- **To be tested on a physical case**



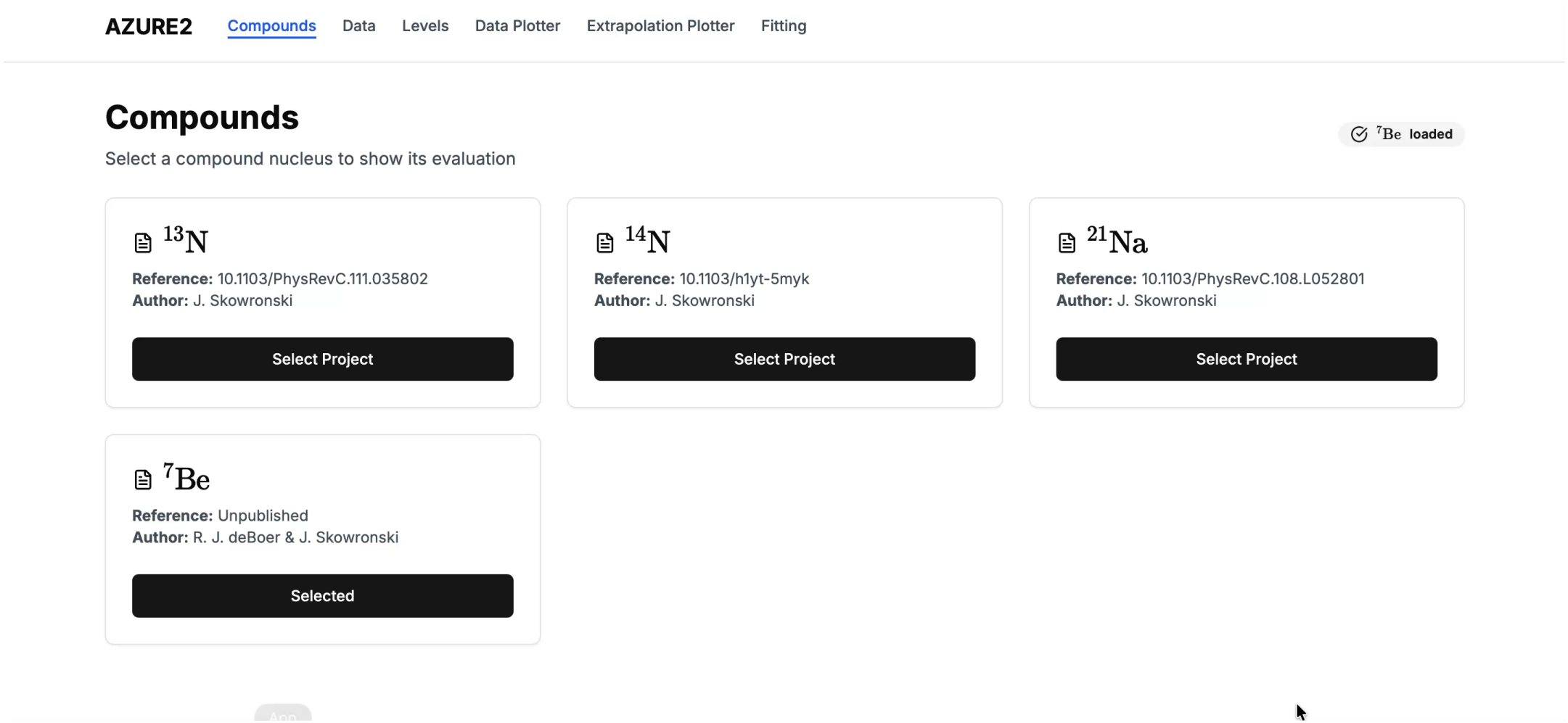
AZURE2: (Bonus) IAEA Integration

In the **Levels and Channels** tab, it is now possible to query automatically the **IAEA database** to **retrieve the excited states**



AZURE2: (Bonus) AZURE2 on the Web

Example available at: http://57.128.201.91:3001



^{7}Be Compound Evaluation

^{7}Be Evaluation with AZURE2

Channels	Separation Energy	Channel Radius
^{3}He + ^{4}He	1.58649 MeV	4.24151 fm
^{6}Li + p	5.6063 MeV	3.94396 fm

Datasets

Abramovich (A0244002)
Elwyn (F0012002/3/5)
Fasoli (D0135002)
Harrison (C1003002)
Ivanovich (A1014010)
McCray (A1410002/3)
Paneru
Schenk (F0049002)
Spiger (A1094004/7)
Tumino (O1221002)

^{7}Be Evaluation with AZURE2

Channels	Separation Energy	Channel Radius
^{3}He + ^{4}He	1.58649 MeV	4.24151 fm
^{6}Li + p	5.6063 MeV	3.94396 fm

- All normalizations were free
- All energy shifts were free (error of **1 keV** assumed for all datasets)

$$\chi^2 = \sum_{i,j} \left[\left(\frac{n_j y_{\mathrm{obs,i}} - y_{\mathrm{theo}}}{n_j \sigma_{\mathrm{stat},i}} \right)^2 + \left(\frac{1 - n_j}{\sigma_{\mathrm{sist},j}} \right)^2 + \left(\frac{\Delta_j}{\Delta_{\mathrm{sist},j}} \right)^2 \right]$$

Datasets

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Ivanovich (A1014010)
McCray (A1410002/3)
Paneru
Schenk (F0049002)
Spiger (A1094004/7)
Tumino (O1221002)

^{7}Be Evaluation with AZURE2

- Best **frequentist fit** reached reduced $\chi^2 = 1.8$
- Covariance matrix calculation **failed**

Datasets

Abramovich (A0244002)
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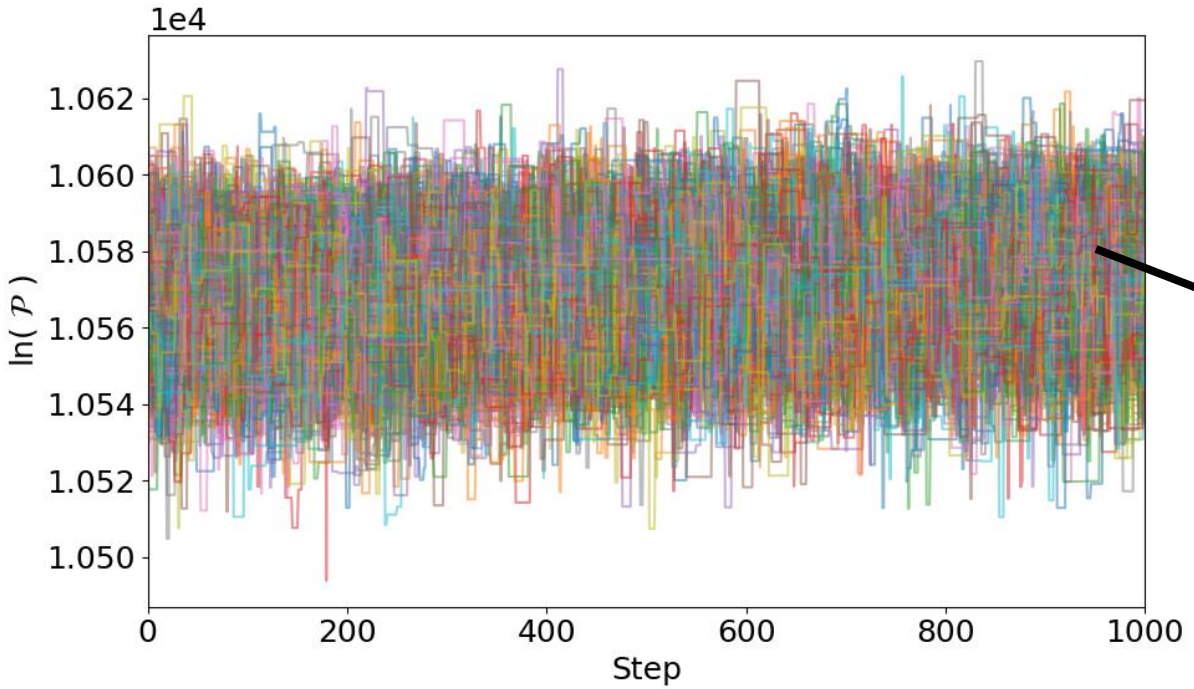
Paneru
Schenk (F0049002)
Spiger (A1094004/7)
Tumino (O1221002)

^{7}Be Evaluation with AZURE2

- Best **frequentist fit** reached reduced $\chi^2 = 1.8$
- Covariance matrix calculation **failed**
- Subsequent **MCMC** evaluation gave reduced $\chi^2 = 1.7$



Approximately 1k samples after burn in used for uncertainty estimation

Datasets

Abramovich (A0244002)
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Paneru
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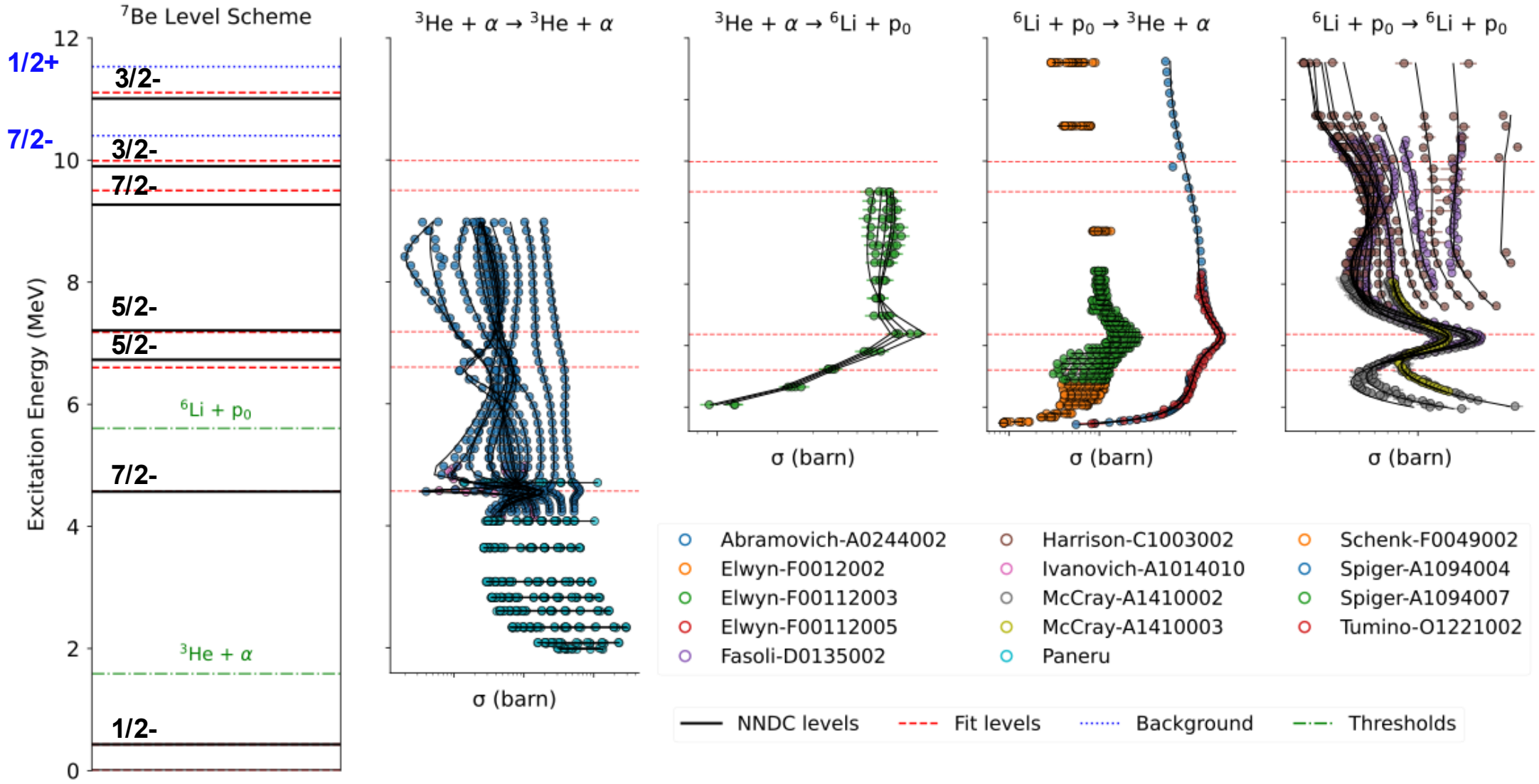
Spiger (A1094004/7)
Tumino (O1221002)

^{7}Be Evaluation with AZURE2: Result



^{7}Be Evaluation with AZURE2: Segments

Datasets

Abramovich (A0244002)
Elwyn (F0012002/3/5)
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McCray (A1410002/3)
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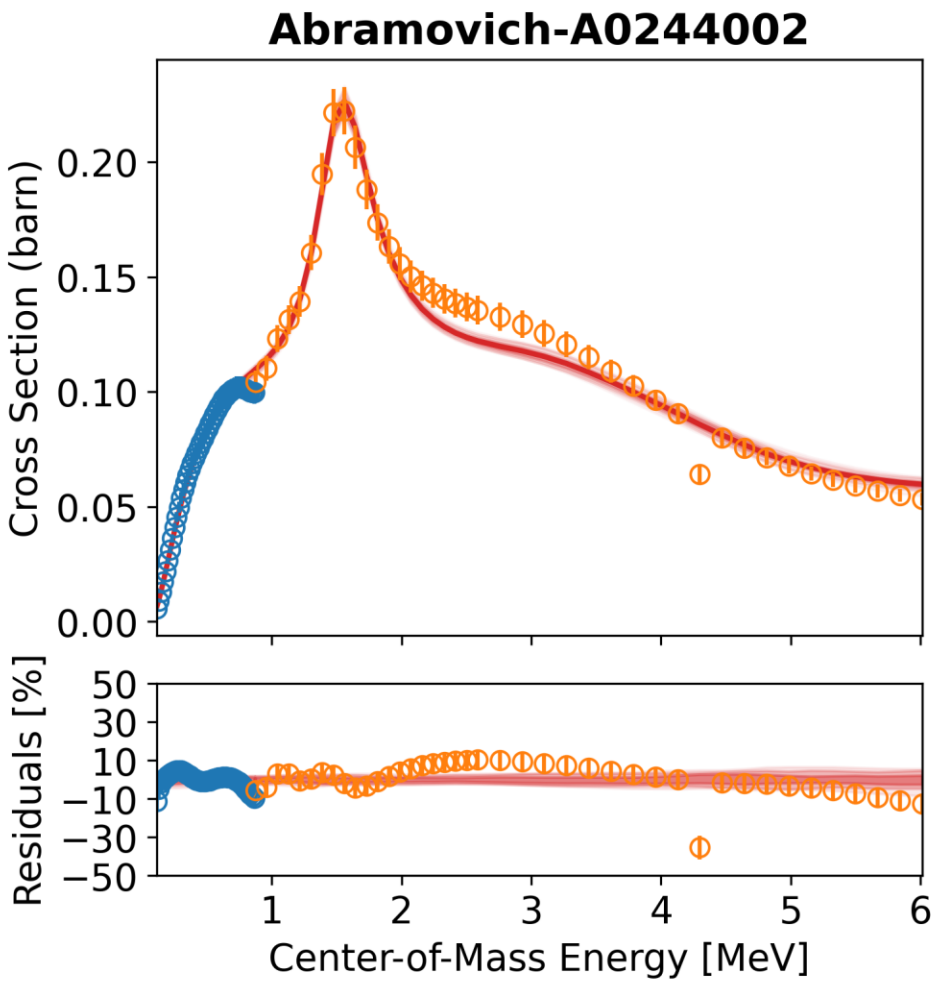

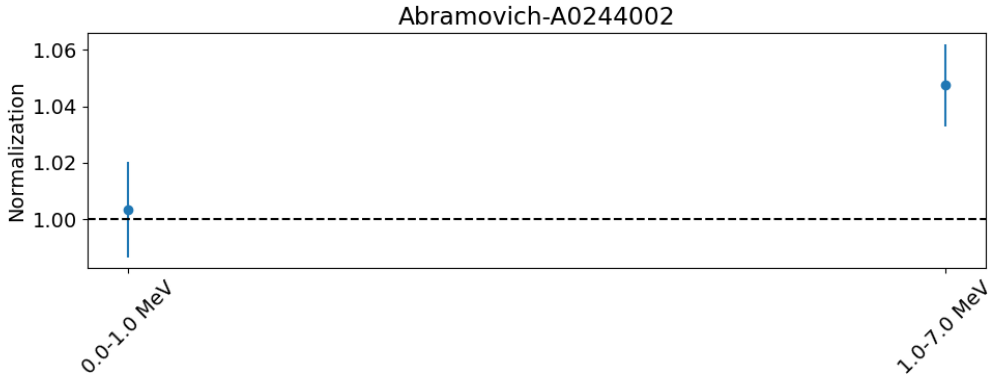

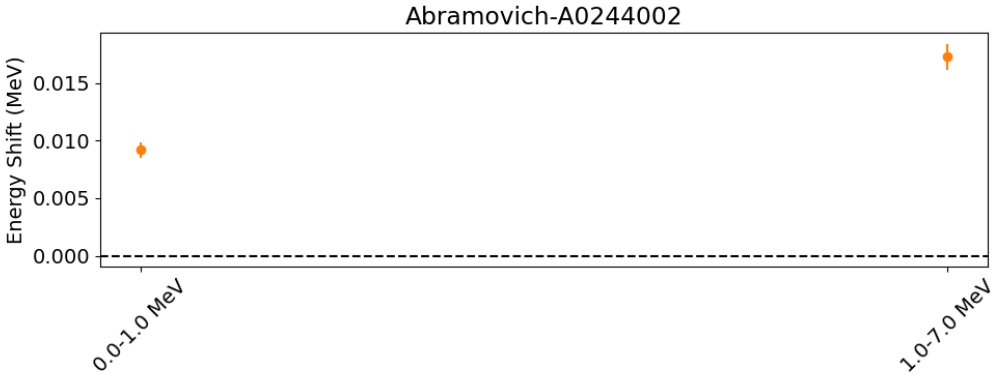

^{7}Be Evaluation with AZURE2: Segments

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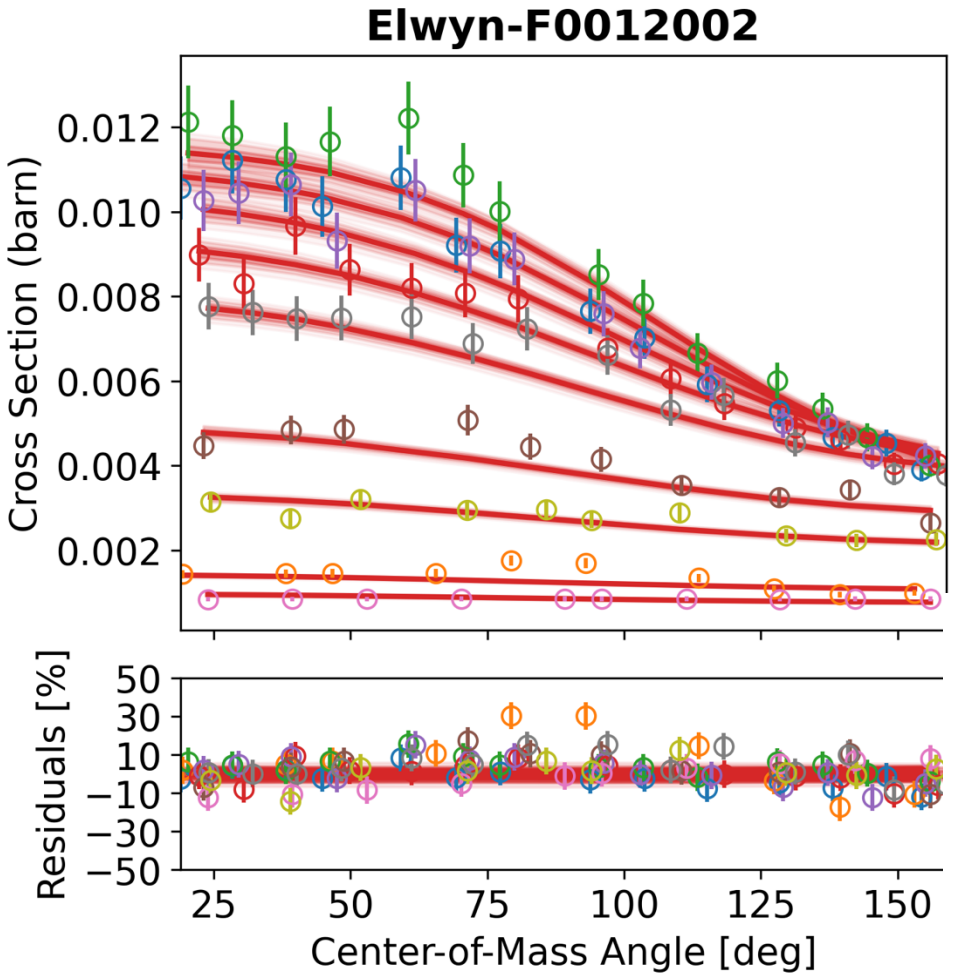

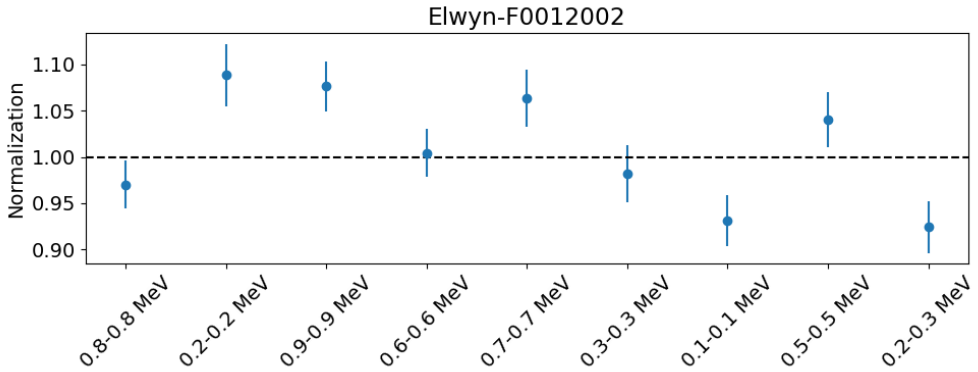

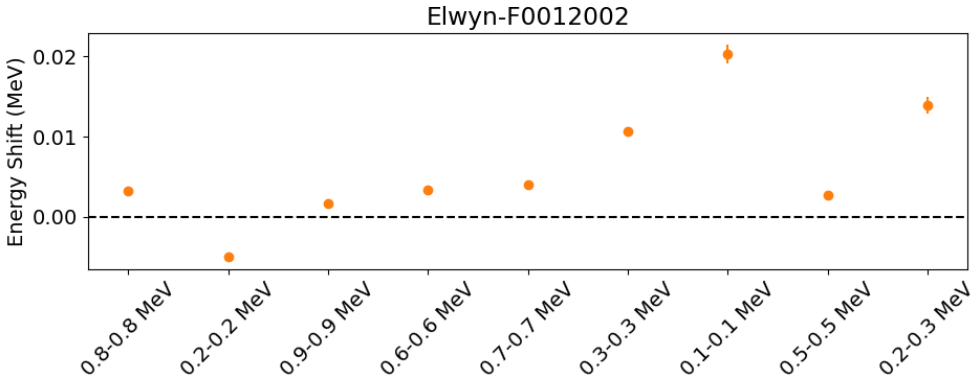

^{7}Be Evaluation with AZURE2: Segments

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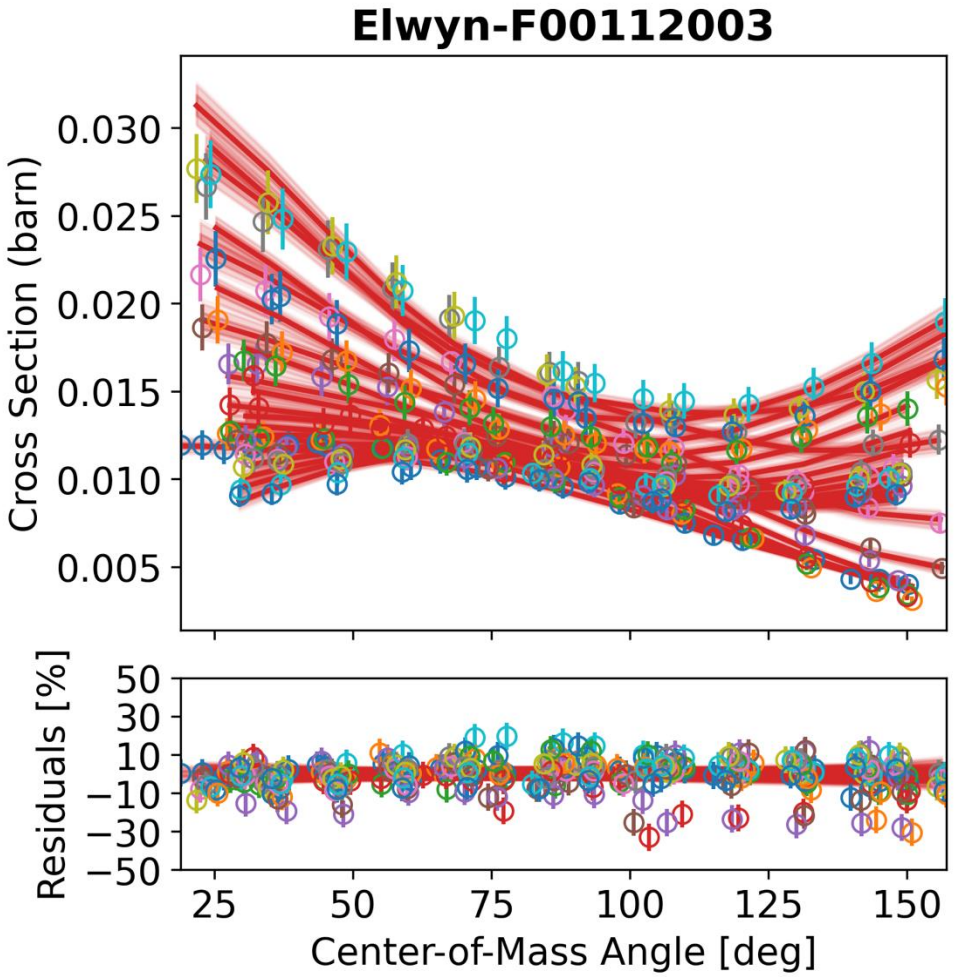

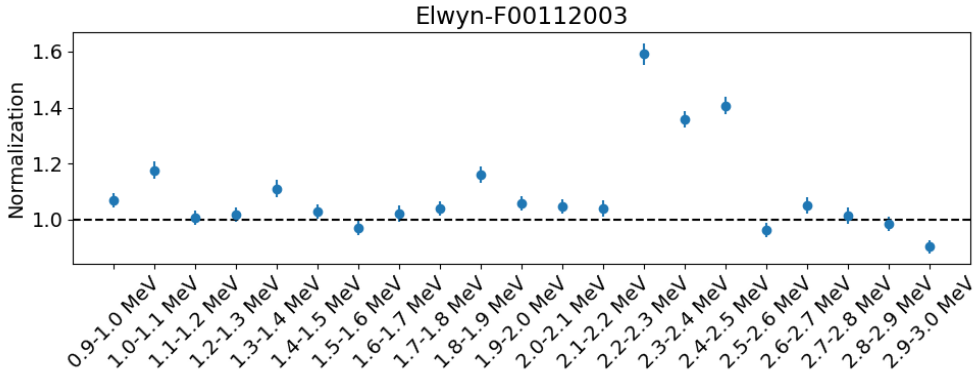

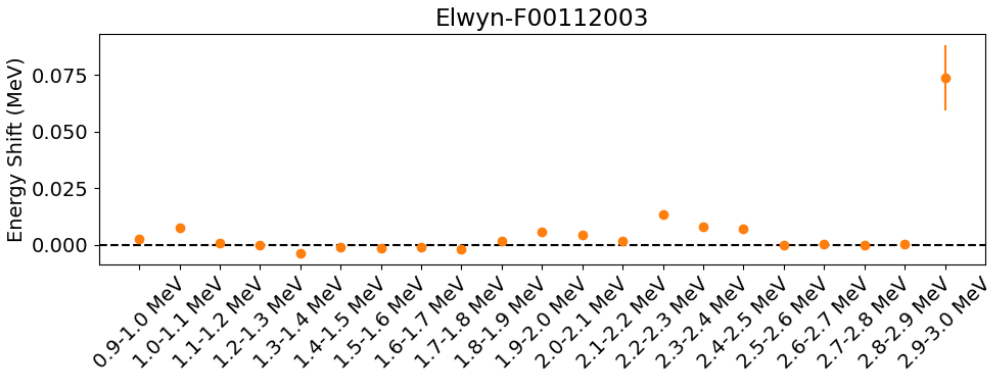

^{7}Be Evaluation with AZURE2: Segments

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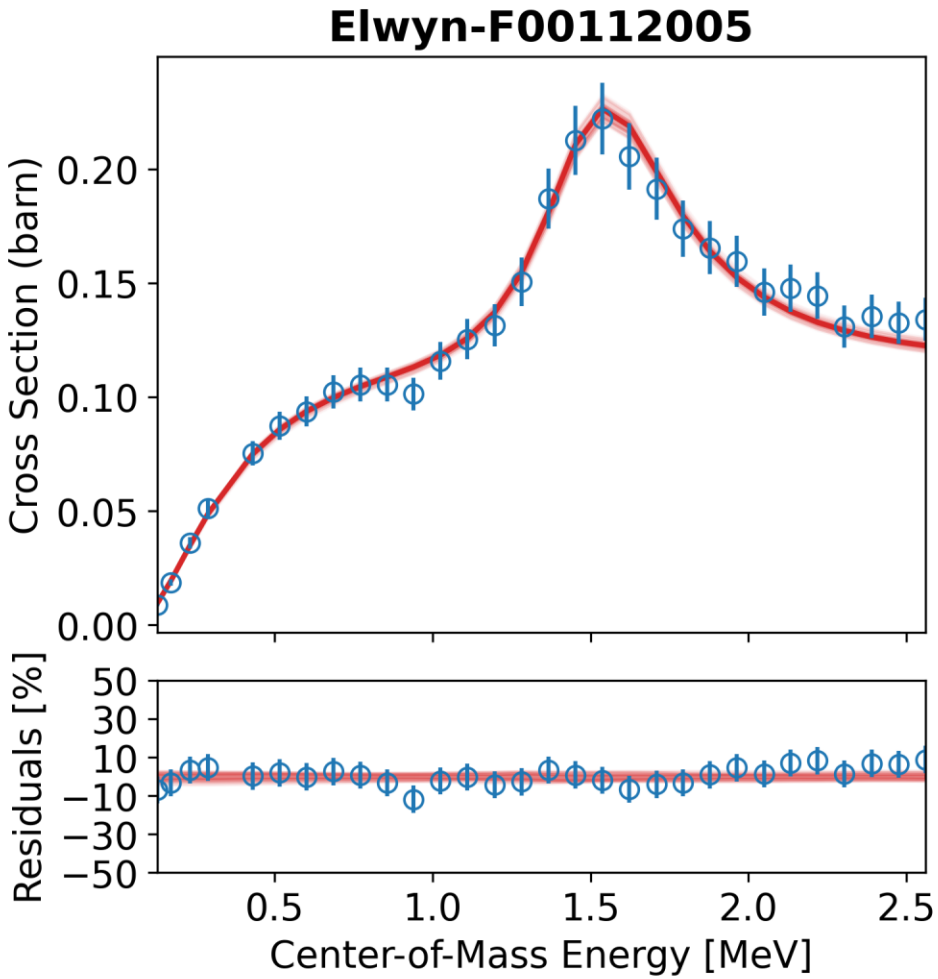

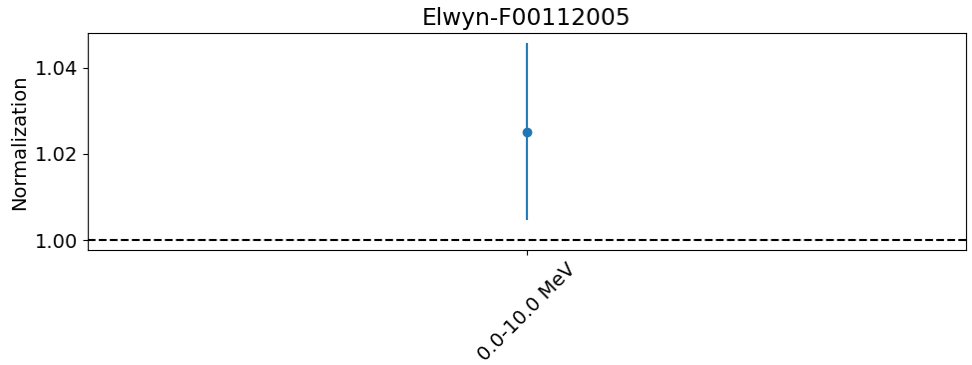

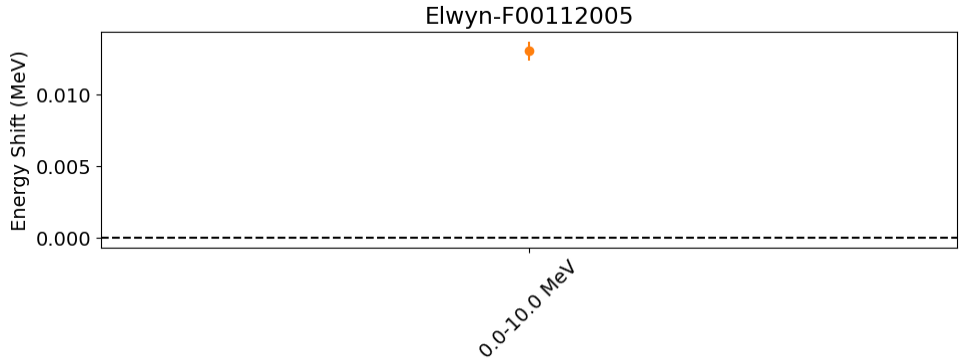

^{7}Be Evaluation with AZURE2: Segments

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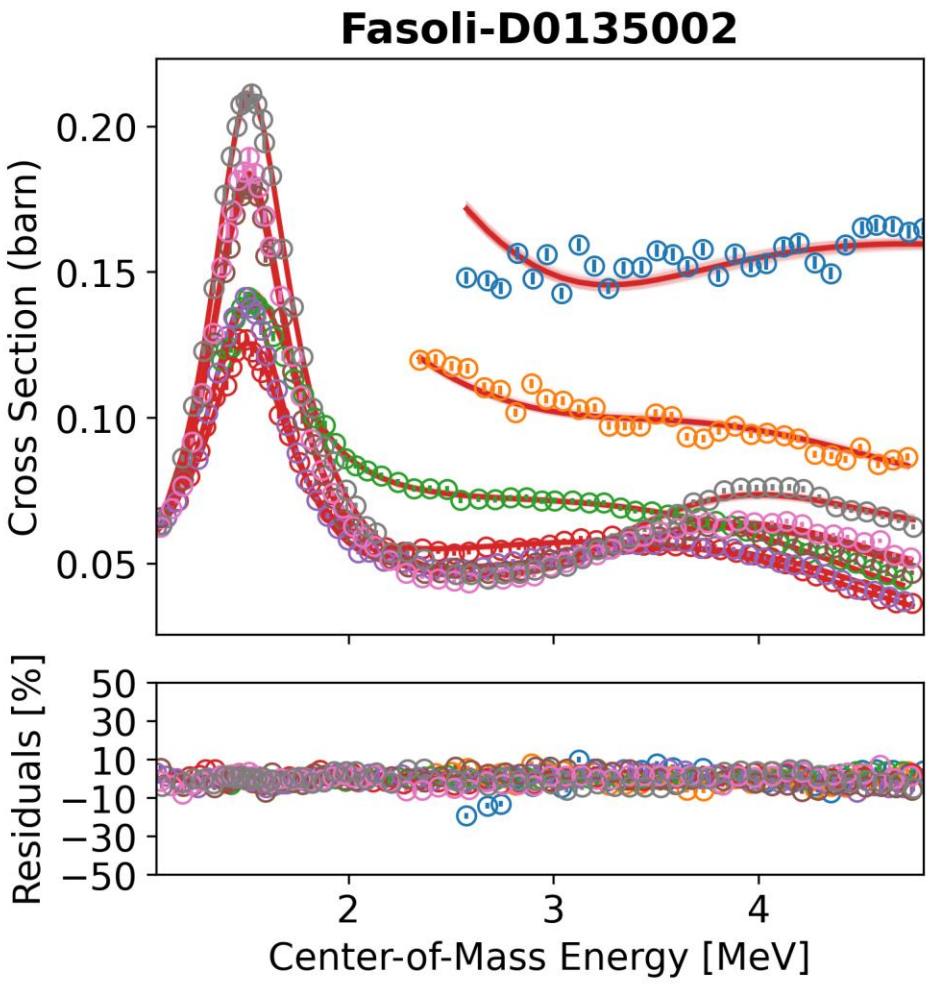

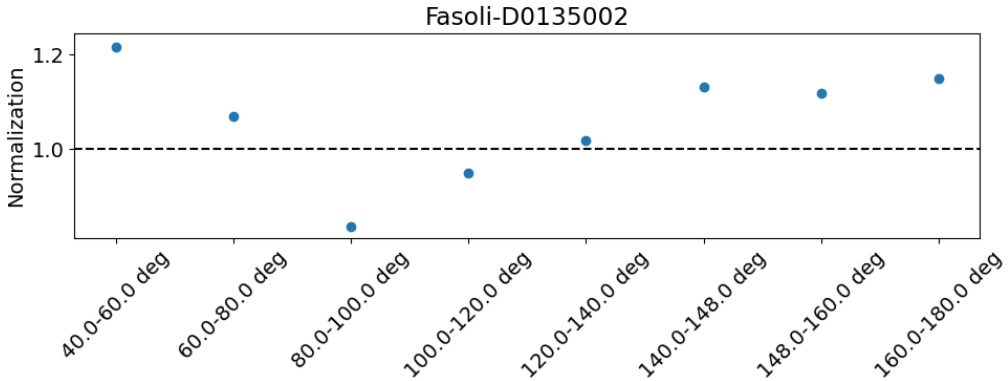

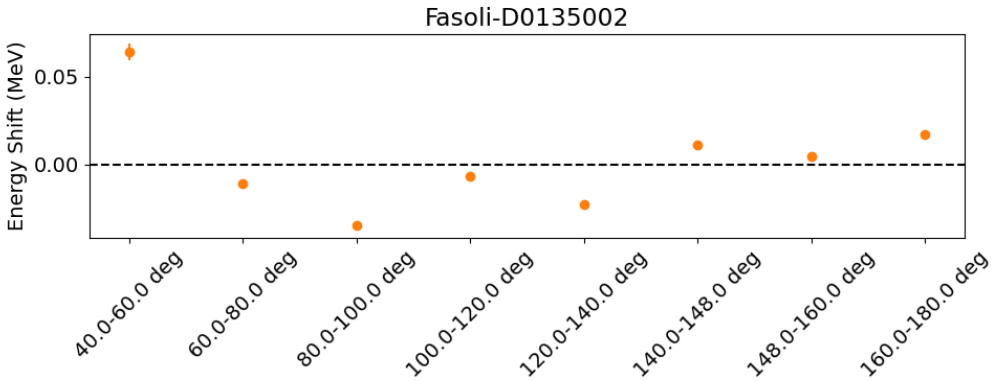

^{7}Be Evaluation with AZURE2: Segments

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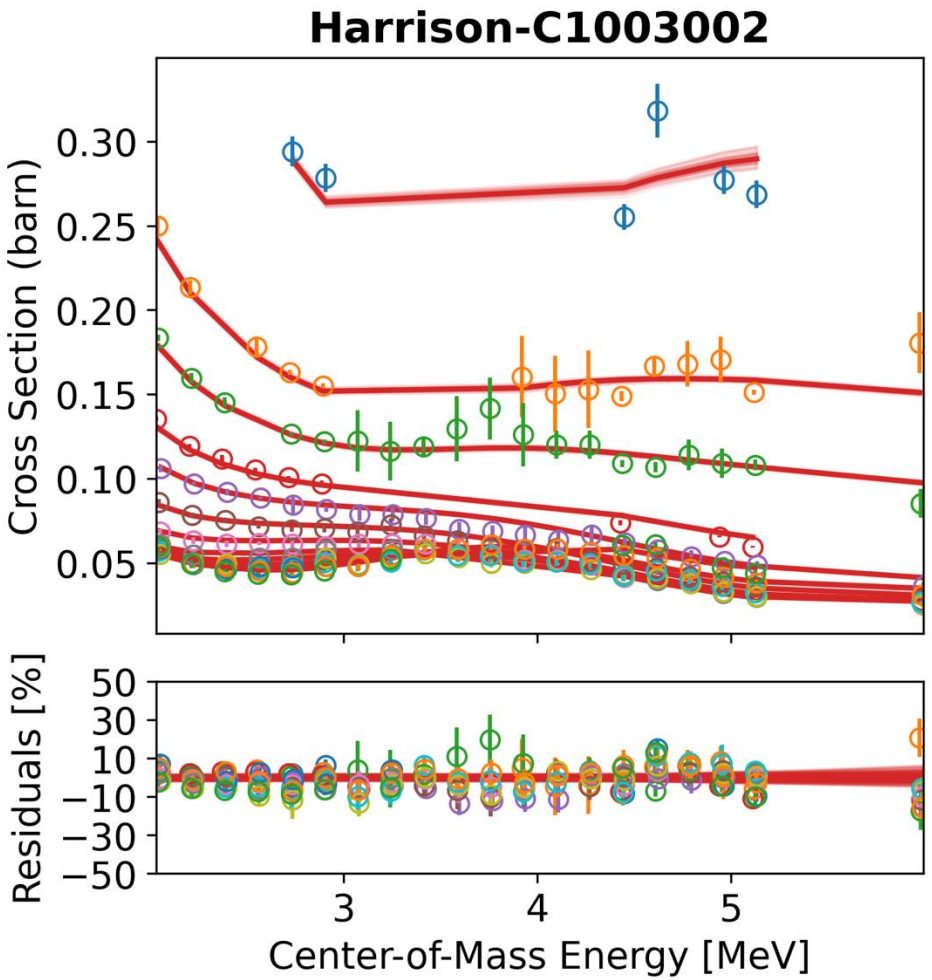

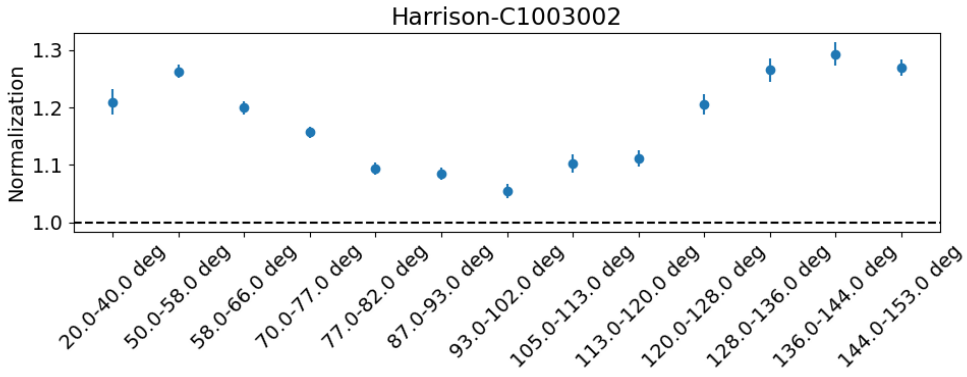

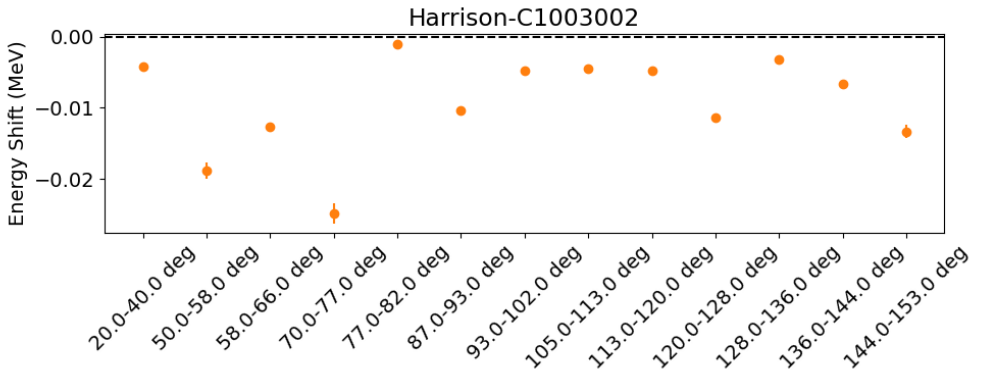

^{7}Be Evaluation with AZURE2: Segments

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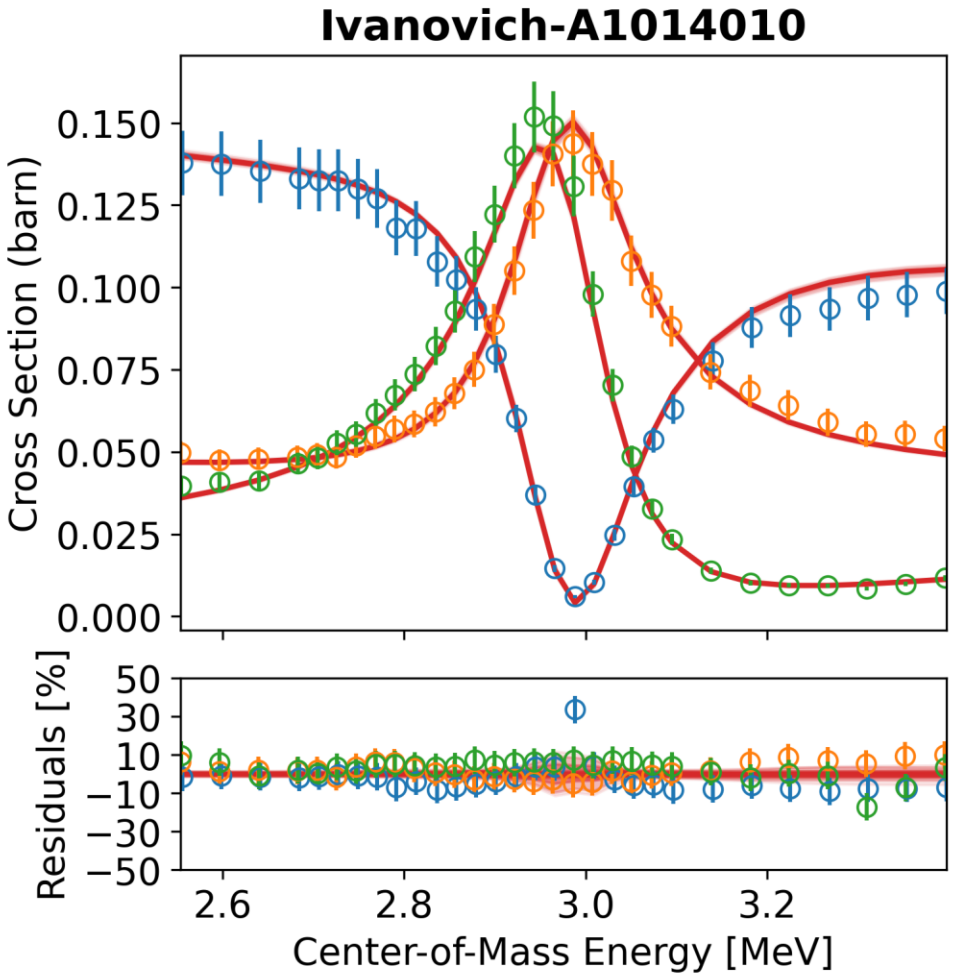

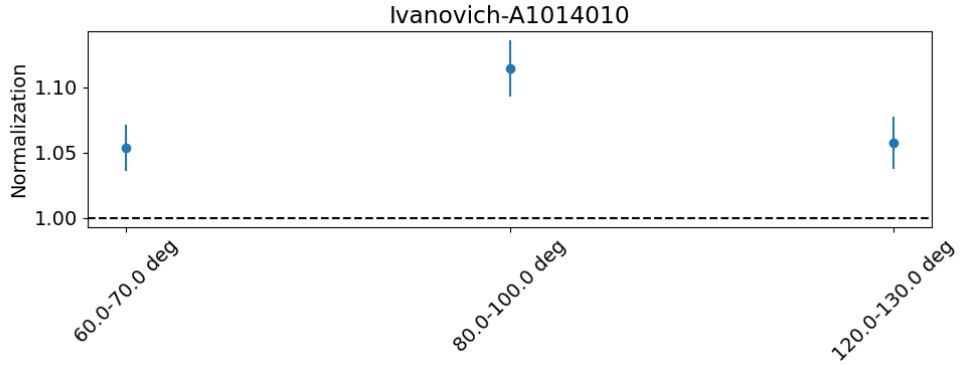

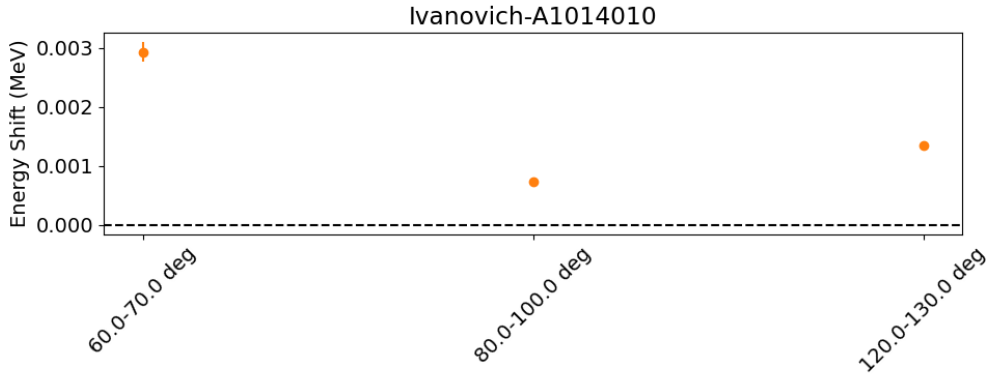

^{7}Be Evaluation with AZURE2: Segments

Datasets

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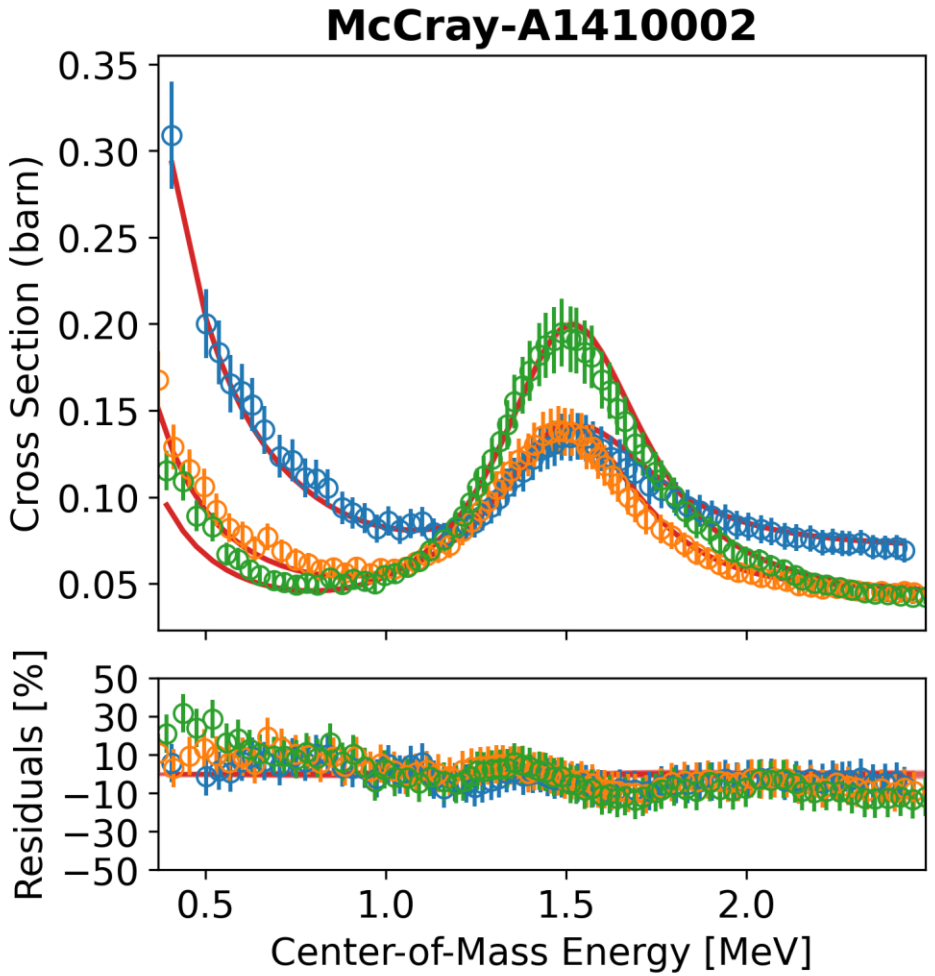

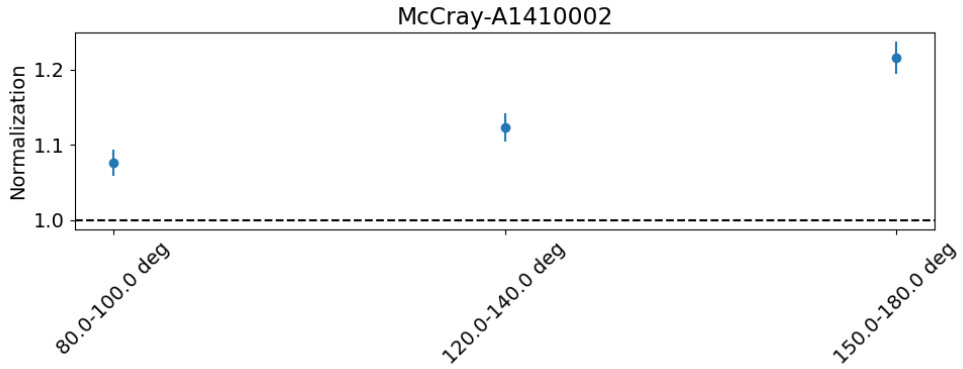

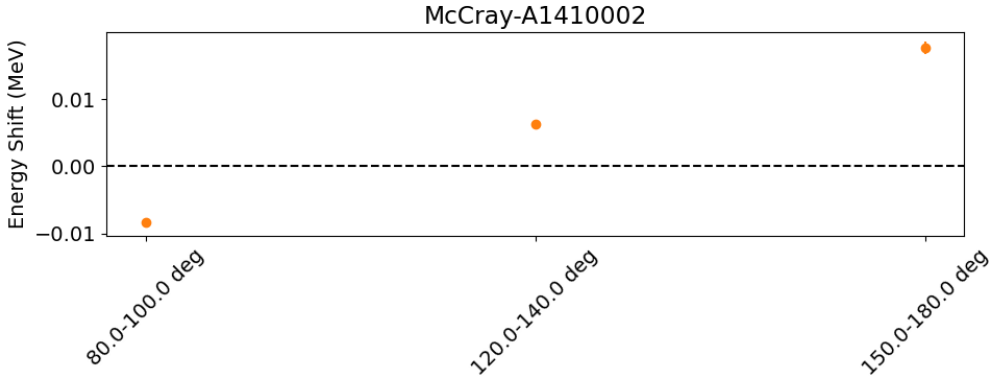

^{7}Be Evaluation with AZURE2: Segments

Datasets

Abramovich (A0244002)
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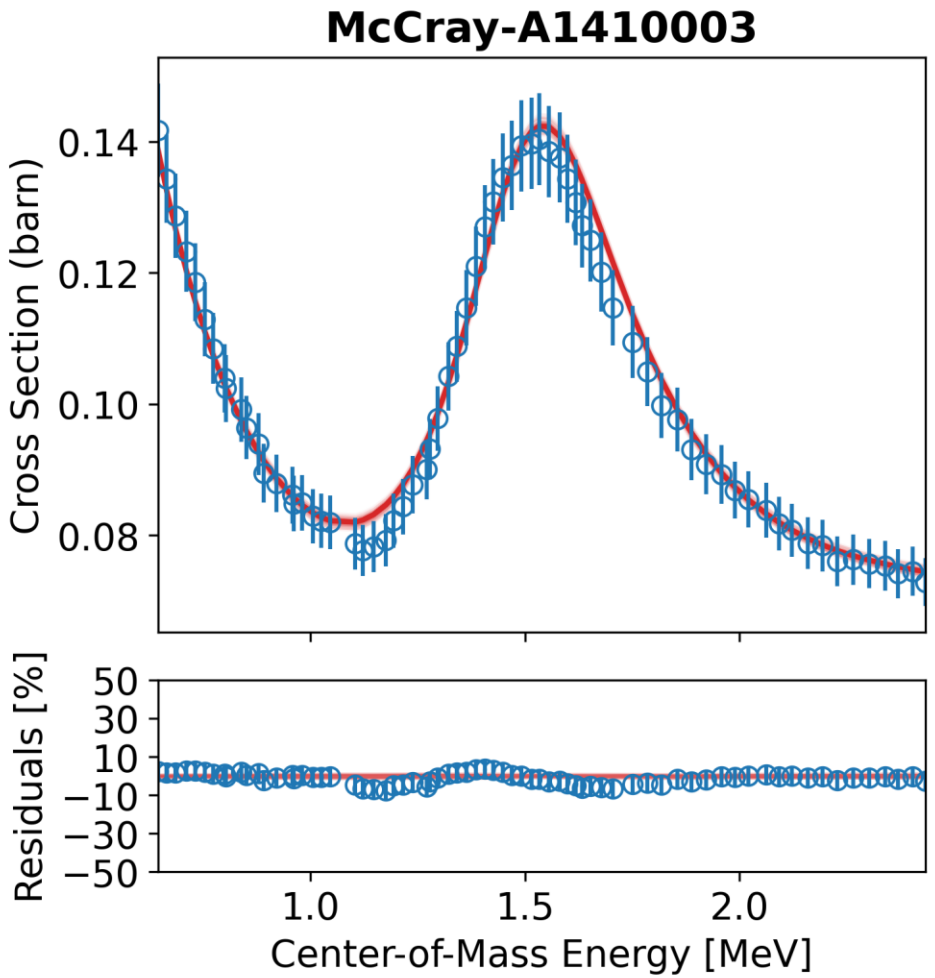

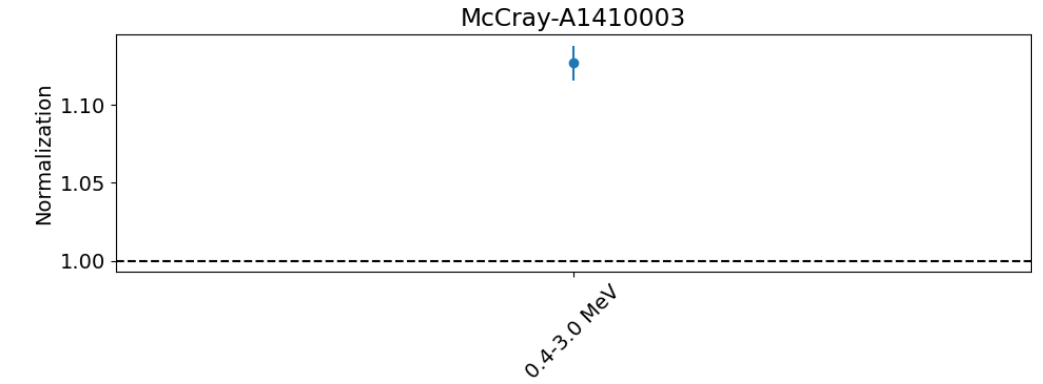

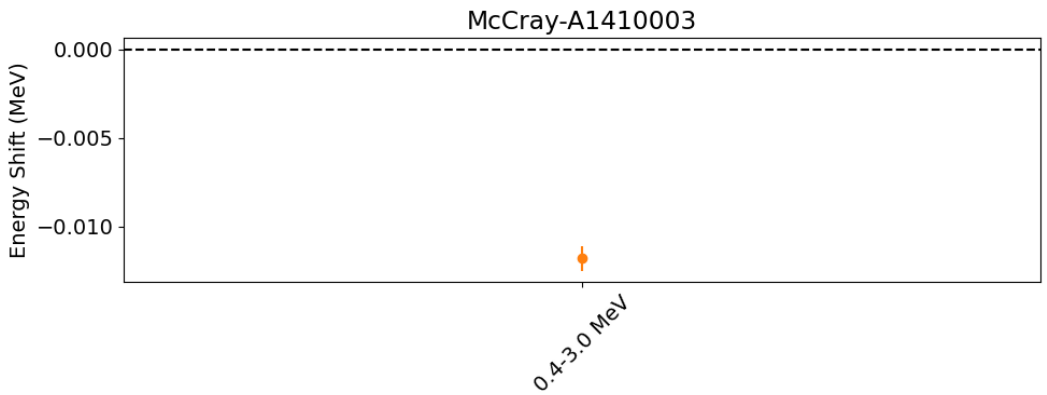

^{7}Be Evaluation with AZURE2: Segments

Datasets

Abramovich (A0244002)
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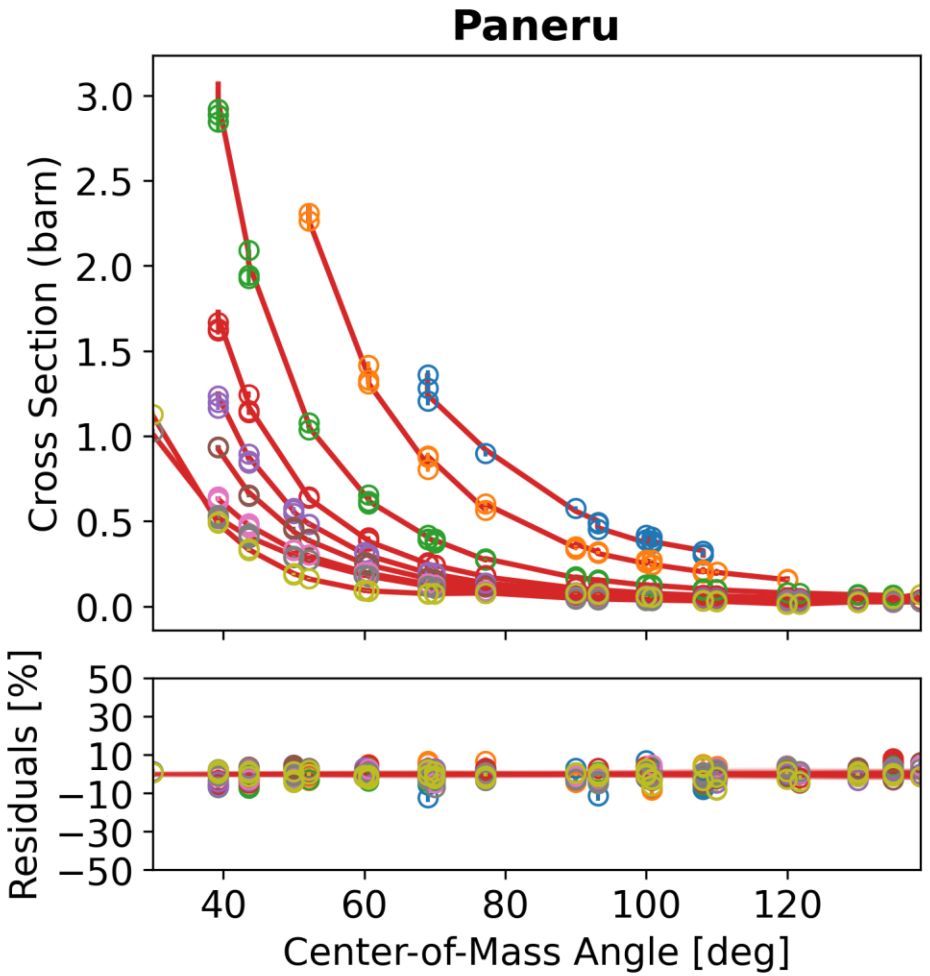

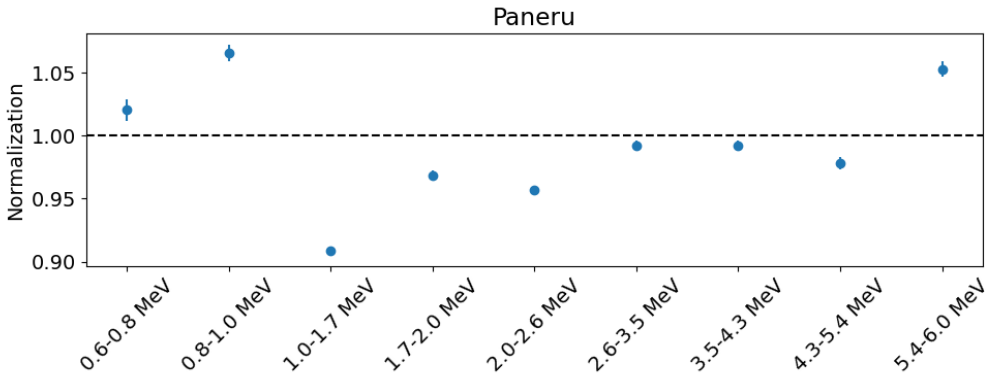

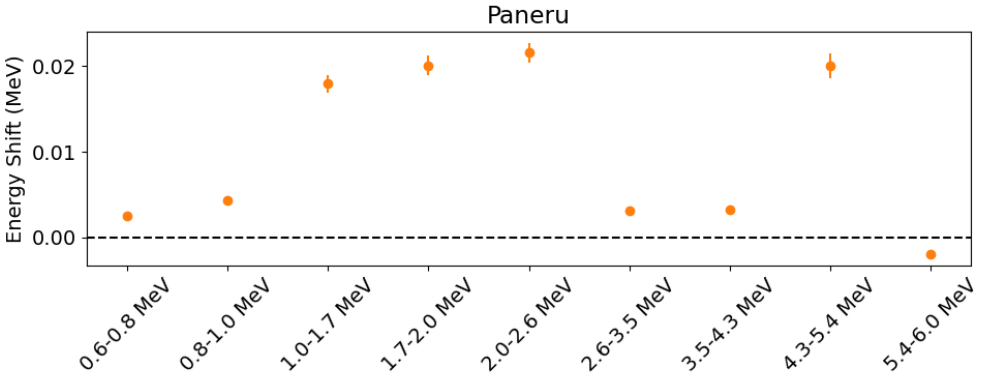

^{7}Be Evaluation with AZURE2: Segments

Datasets

Abramovich (A0244002)
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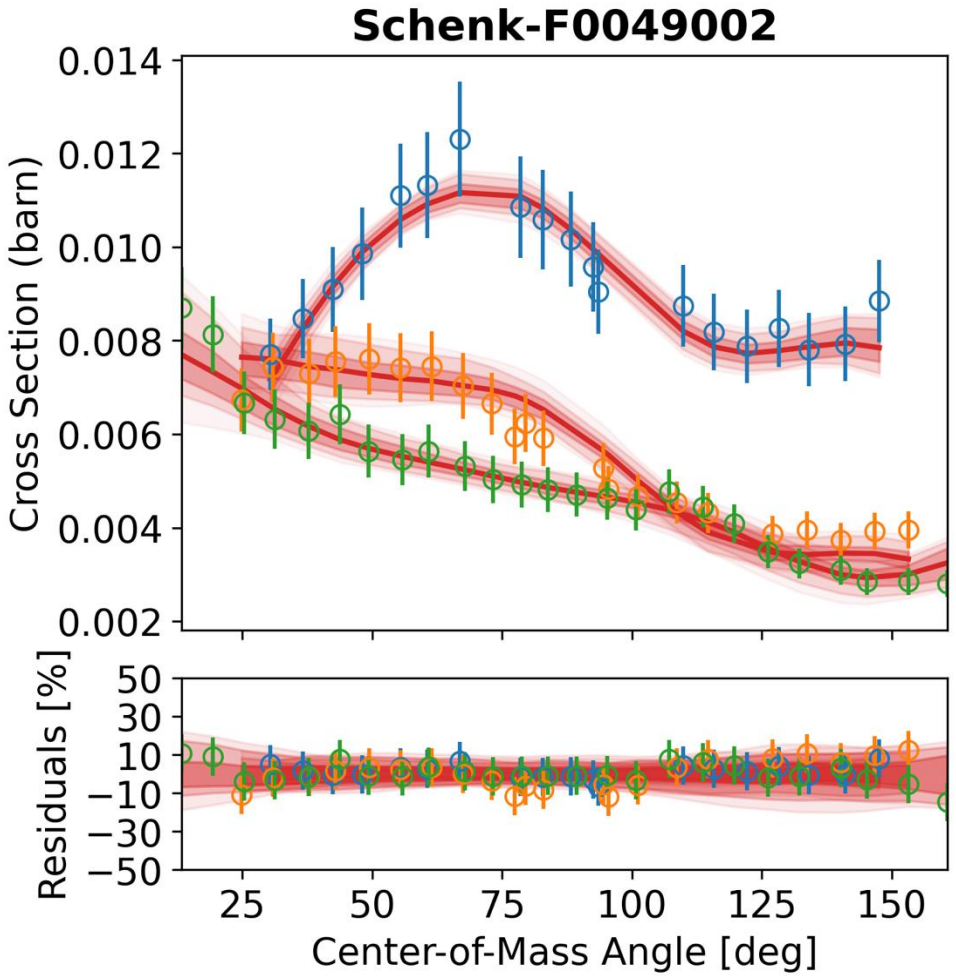

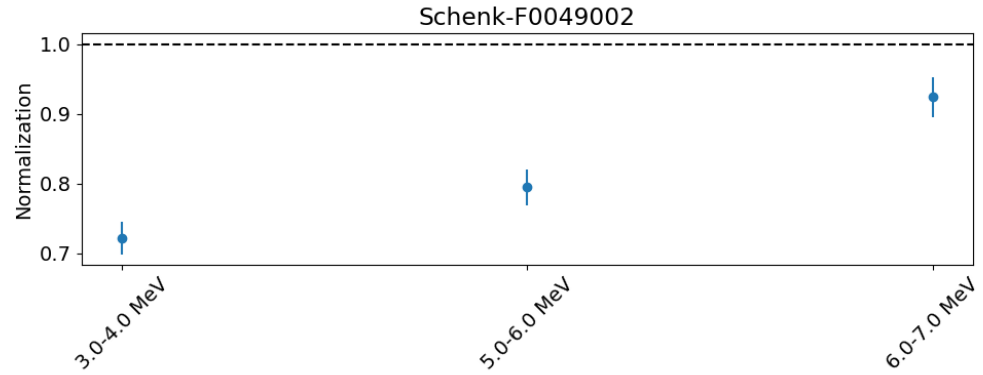

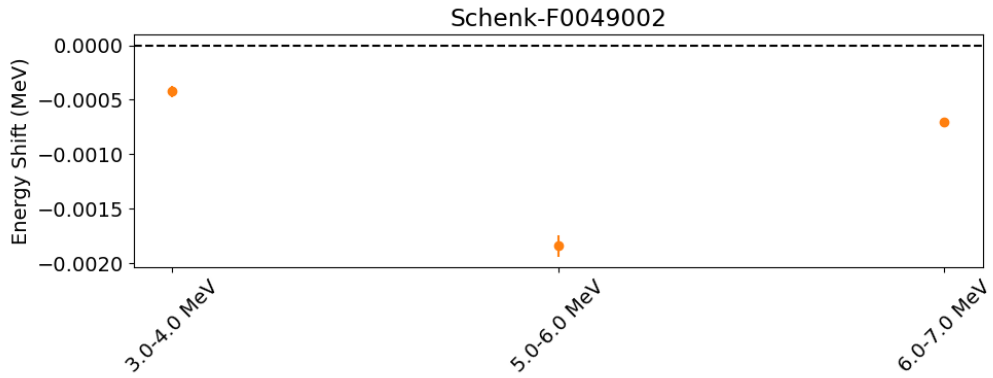

^{7}Be Evaluation with AZURE2: Segments

Datasets

Abramovich (A0244002)
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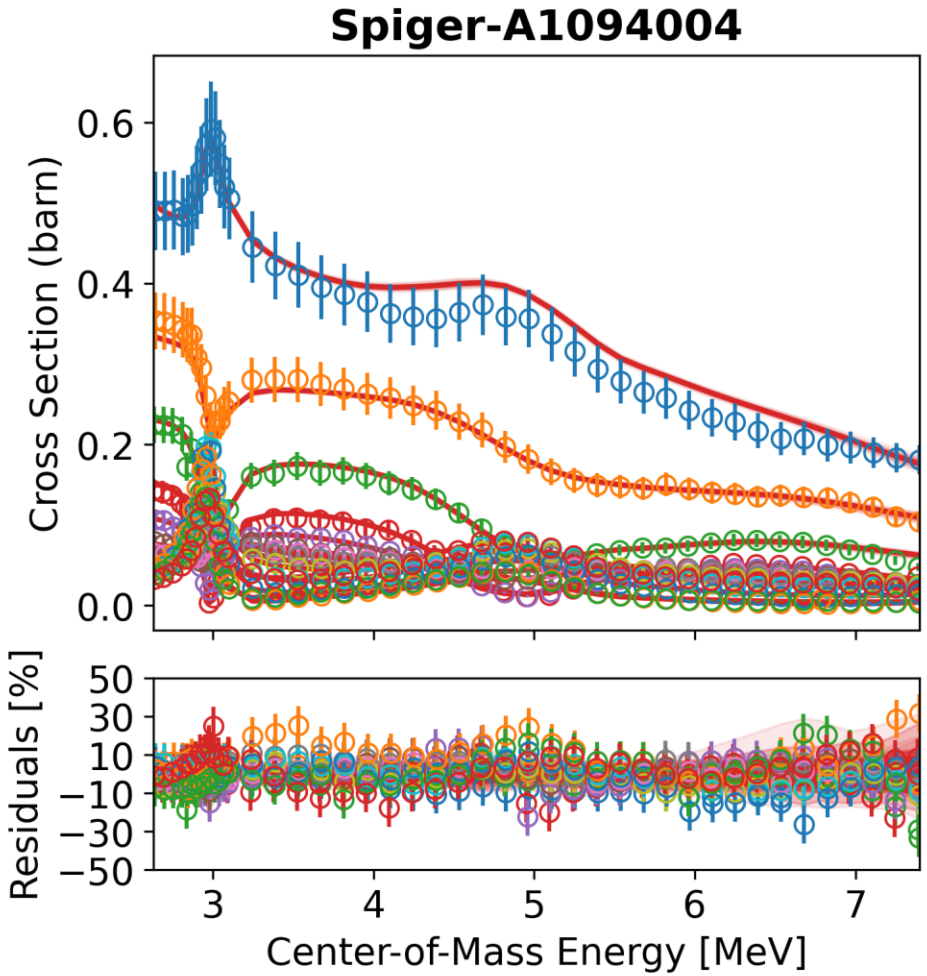

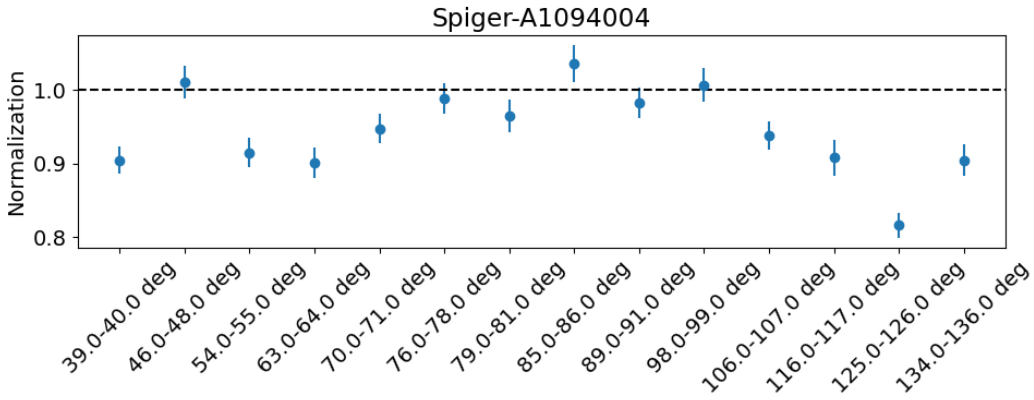

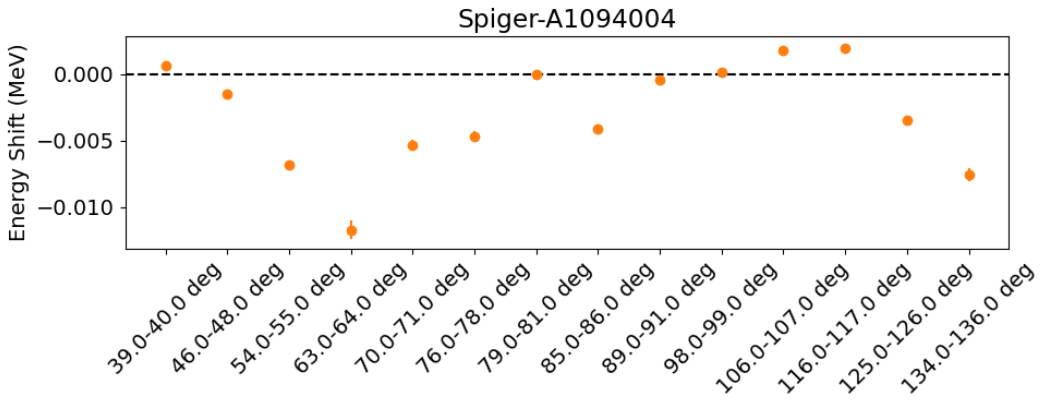

^{7}Be Evaluation with AZURE2: Segments

Datasets

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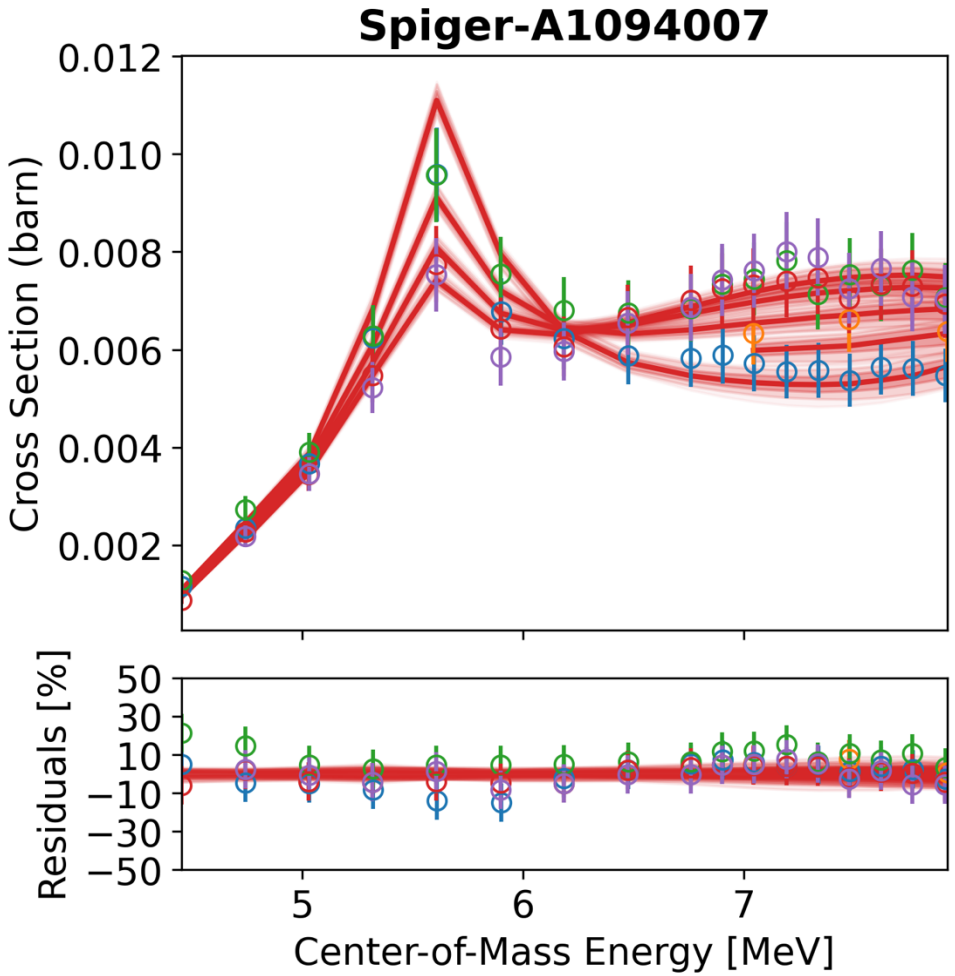
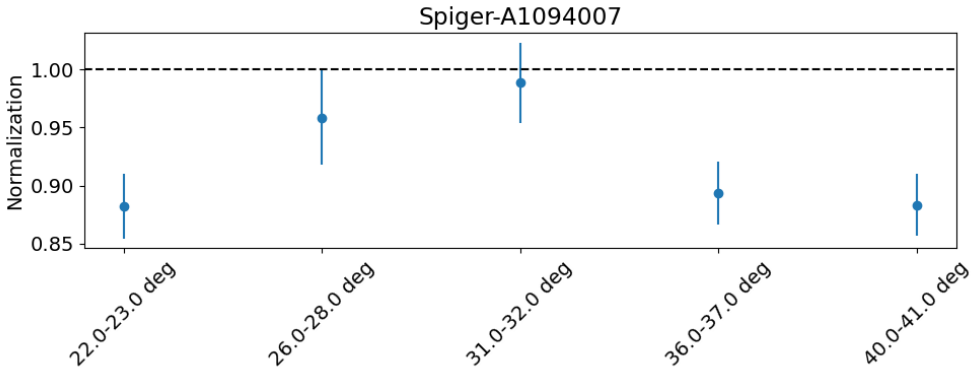
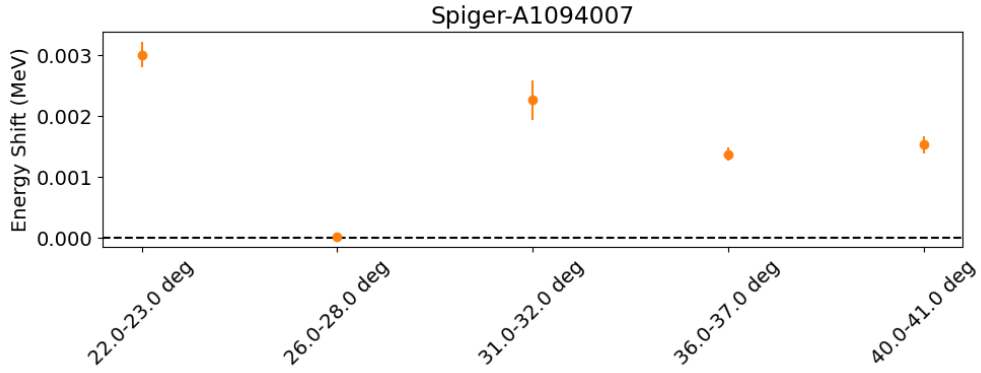
Tumino (O1221002)



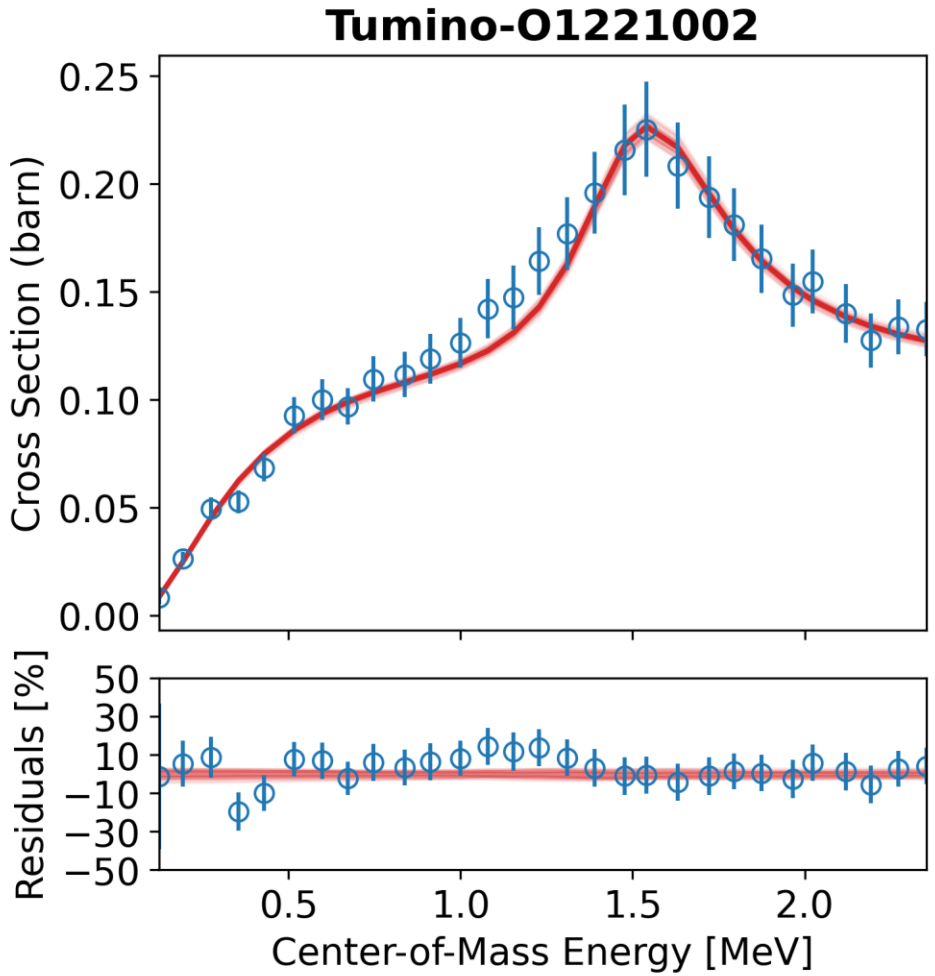


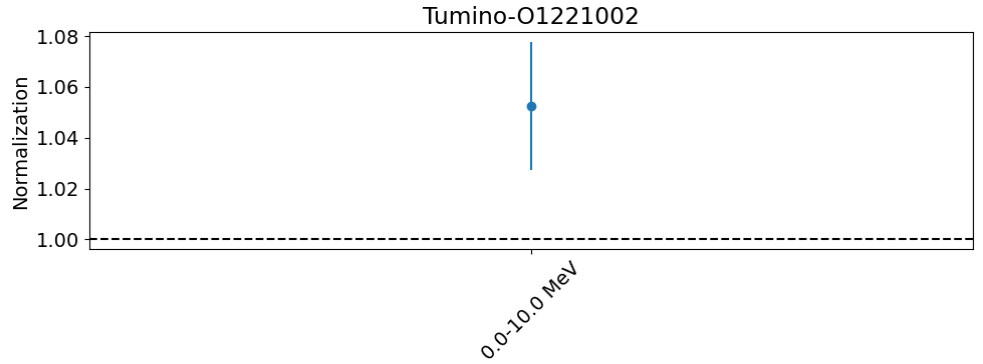


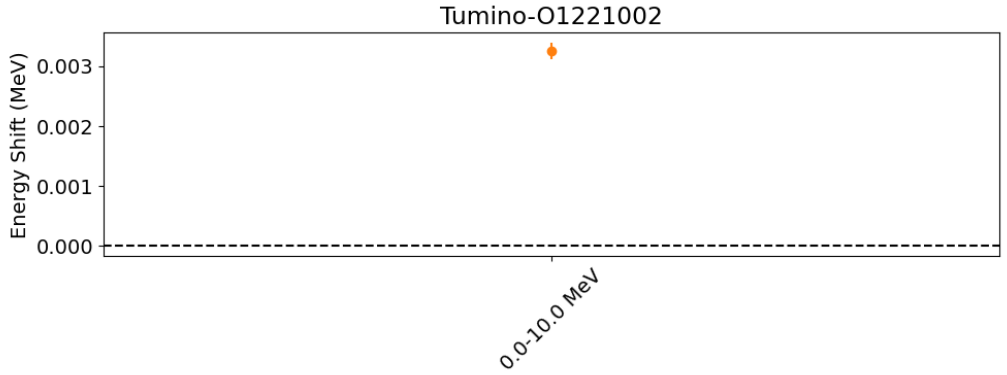
^{7}Be Evaluation with AZURE2: Segments

Datasets

Abramovich (A0244002)
Elwyn (F0012002/3/5)
Fasoli (D0135002)
Harrison (C1003002)
Ivanovich (A1014010)
McCray (A1410002/3)
Paneru
Schenk (F0049002)
Spiger (A1094004/7)
Tumino (O1221002)







Conclusions

- In the last year AZURE2 got a lot of upgrades: **testing** and **paper in progress**
- The ^{7}Be evaluation is ready and reasonable: however, **background levels are needed**
- Maybe trying the **Hybrid Potential** model could help reducing the background dependency?

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Thank you for attention!