

AZURE2 Development Status and ^7Be Compound Evaluation

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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

AZURE2 -- /Users/kuba/Desktop/R-Matrix/IAEA/evaluations/7Be/AZURE2/7Be.azr

Particle Pairs Levels and Channels Segments Experimental Effects **Fitting Settings** Calculate MCMC Plot

Level Parameters Normalization Energy Shifts

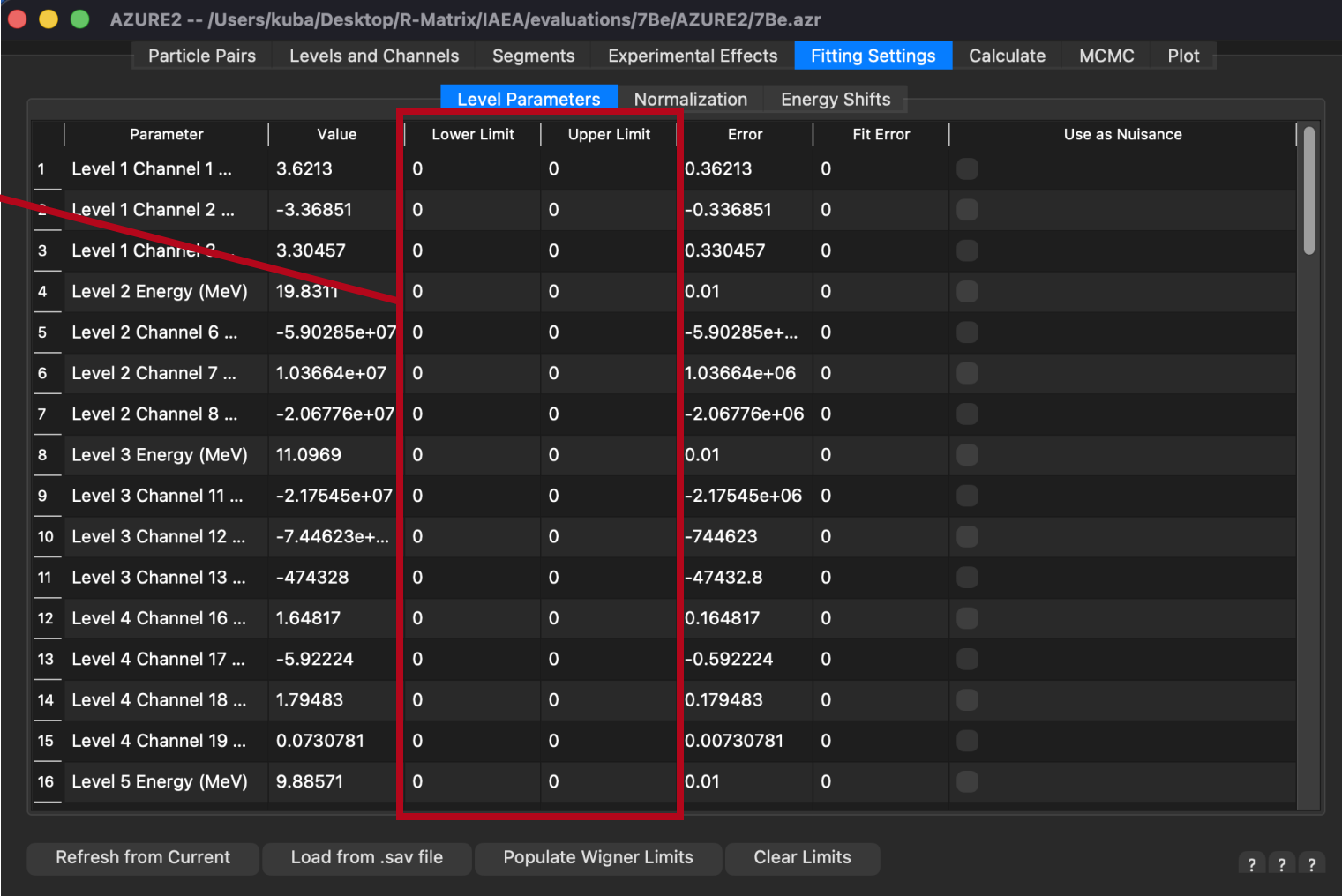
	Parameter	Value	Lower Limit	Upper Limit	Error	Fit Error	Use as Nuisance
1	Level 1 Channel 1 ...	3.6213	0	0	0.36213	0	☐
2	Level 1 Channel 2 ...	-3.36851	0	0	-0.336851	0	☐
3	Level 1 Channel 3 ...	3.30457	0	0	0.330457	0	☐
4	Level 2 Energy (MeV)	19.8311	0	0	0.01	0	☐
5	Level 2 Channel 6 ...	-5.90285e+07	0	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	☐

Refresh from Current Load from .sav file Populate Wigner Limits Clear Limits

? ? ?

AZURE2: Fitting Tab

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



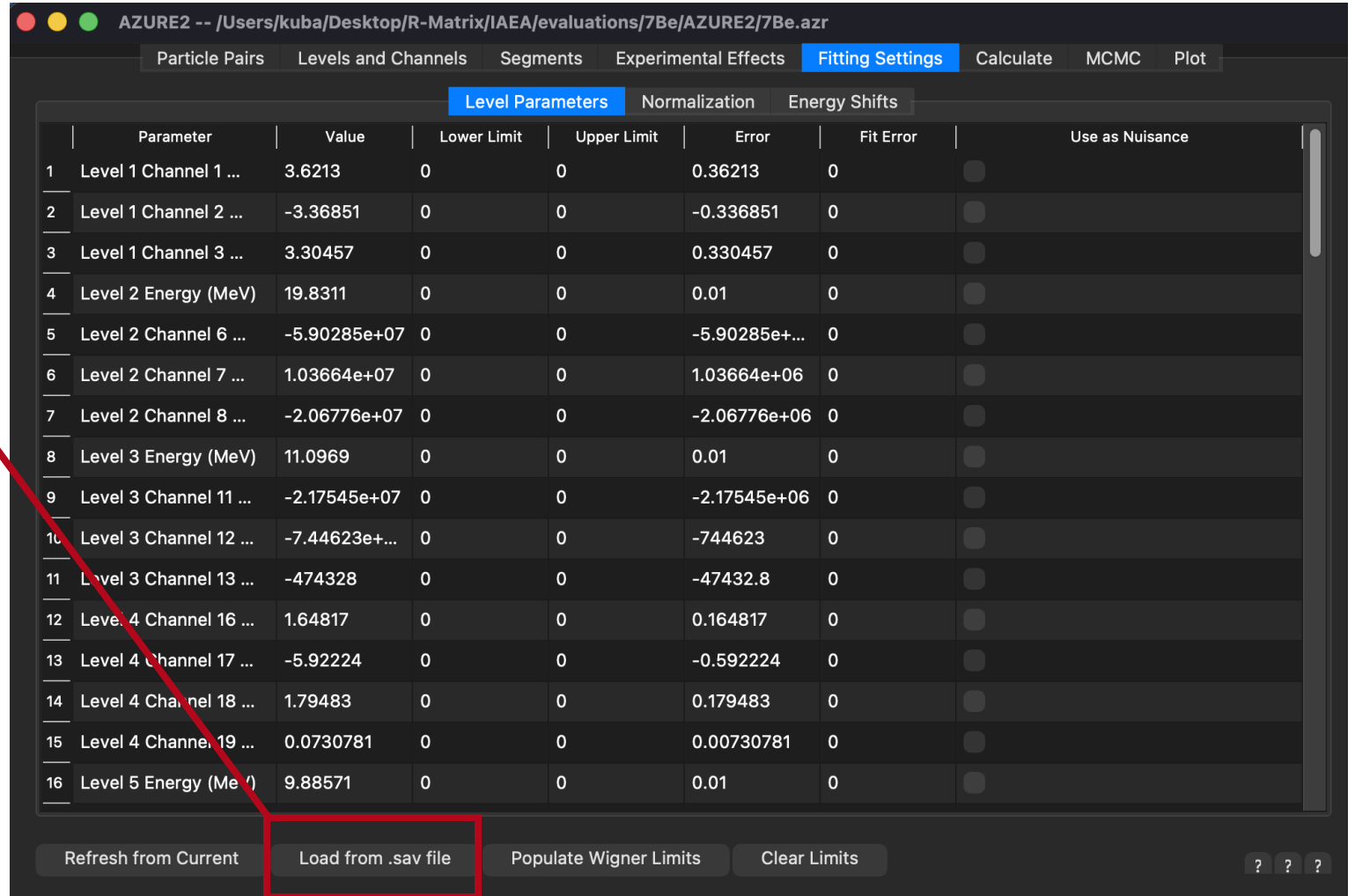
The screenshot shows the AZURE2 software interface with the 'Fitting Settings' tab selected. The 'Level Parameters' section is highlighted with a red box. A red arrow points to the 'Lower Limit' and 'Upper Limit' columns, indicating the possibility of adding limits for each parameter.

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15	Level 4 Channel 19 ...	0.0730781	0	0	0.00730781	0	☐
16	Level 5 Energy (MeV)	9.88571	0	0	0.01	0	☐

Buttons at the bottom: Refresh from Current, Load from .sav file, Populate Wigner Limits, Clear Limits, and three question marks.

AZURE2: Fitting Tab

- Possibility of adding **lower** and **upper limits** for each parameter
- **Update** of the AZURE2 file with the best-fit parameters



AZURE2 -- /Users/kuba/Desktop/R-Matrix/IAEA/evaluations/7Be/AZURE2/7Be.azr

Particle Pairs Levels and Channels Segments Experimental Effects **Fitting Settings** Calculate MCMC Plot

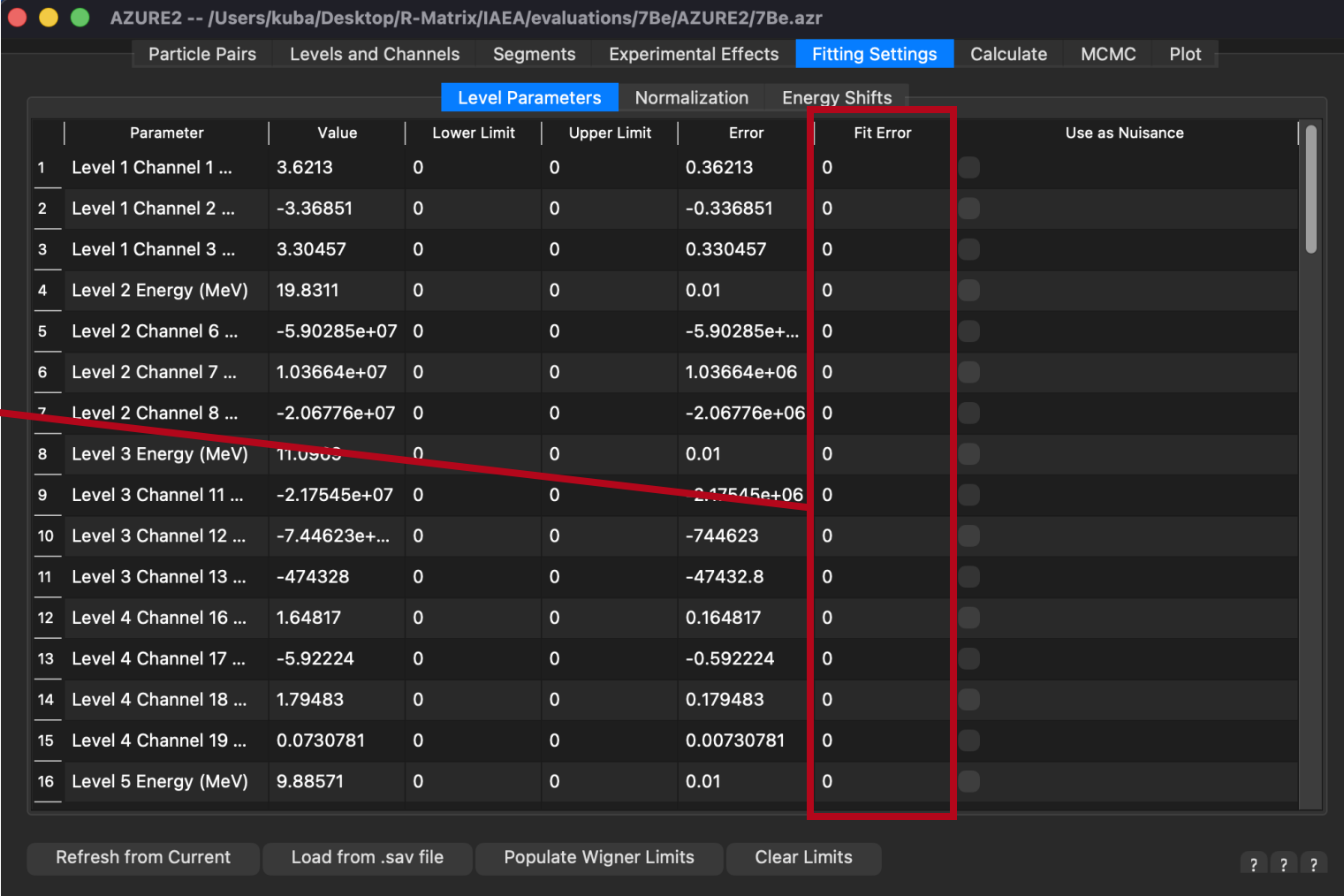
Level Parameters Normalization Energy Shifts

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Refresh from Current Load from .sav file Populate Wigner Limits Clear Limits ? ? ?

AZURE2: Fitting Tab

- Possibility of adding **lower** and **upper limits** for each parameter
- **Update** of the AZURE2 file with the best-fit parameters
- **Fit error** visualization



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AZURE2: Fitting Tab

- Possibility of adding **lower** and **upper limits** for each parameter
- **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 -- /Users/kuba/Desktop/R-Matrix/IAEA/evaluations/7Be/AZURE2/7Be.azr

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Refresh from Current Load from .sav file Populate Wigner Limits Clear Limits ? ? ?

AZURE2: Wigner Limits

The **Wigner Limits** are calculated as:

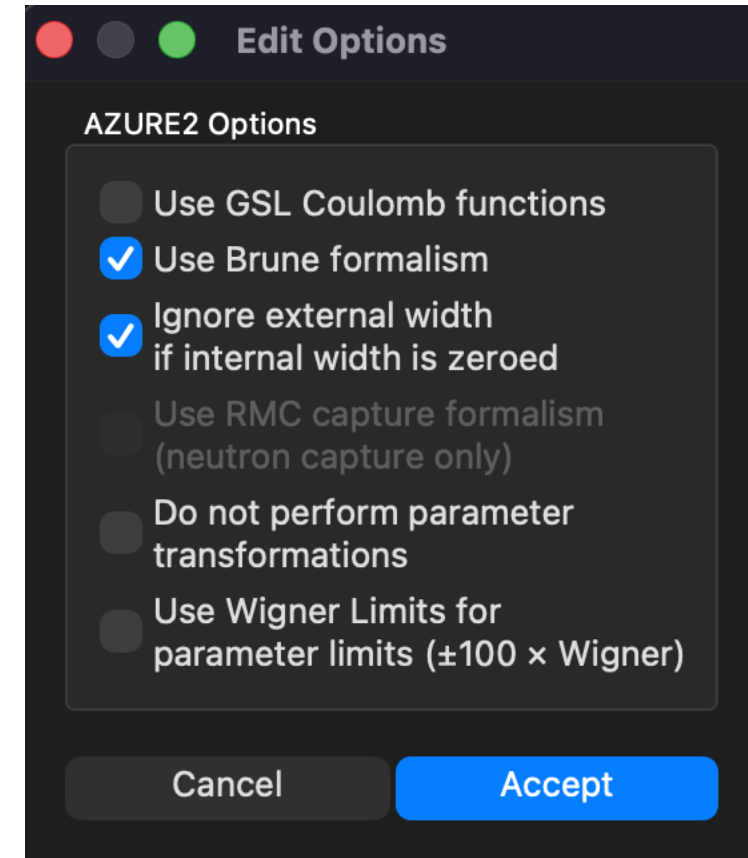
$$\gamma_W^2 = \frac{3\hbar^2}{2\mu a^2}$$

μ : reduced mass

a : channel radius

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

AZURE2 → Configure → Runtime Options



AZURE2: Wigner Limits

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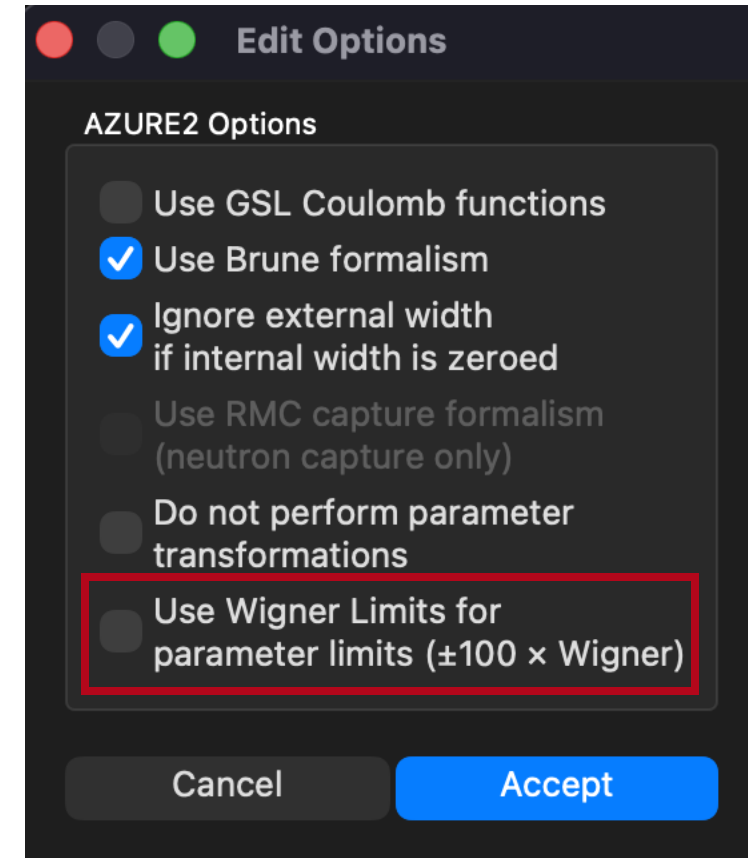
μ : reduced mass

a : channel radius

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

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

AZURE2 → Configure → Runtime Options



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**

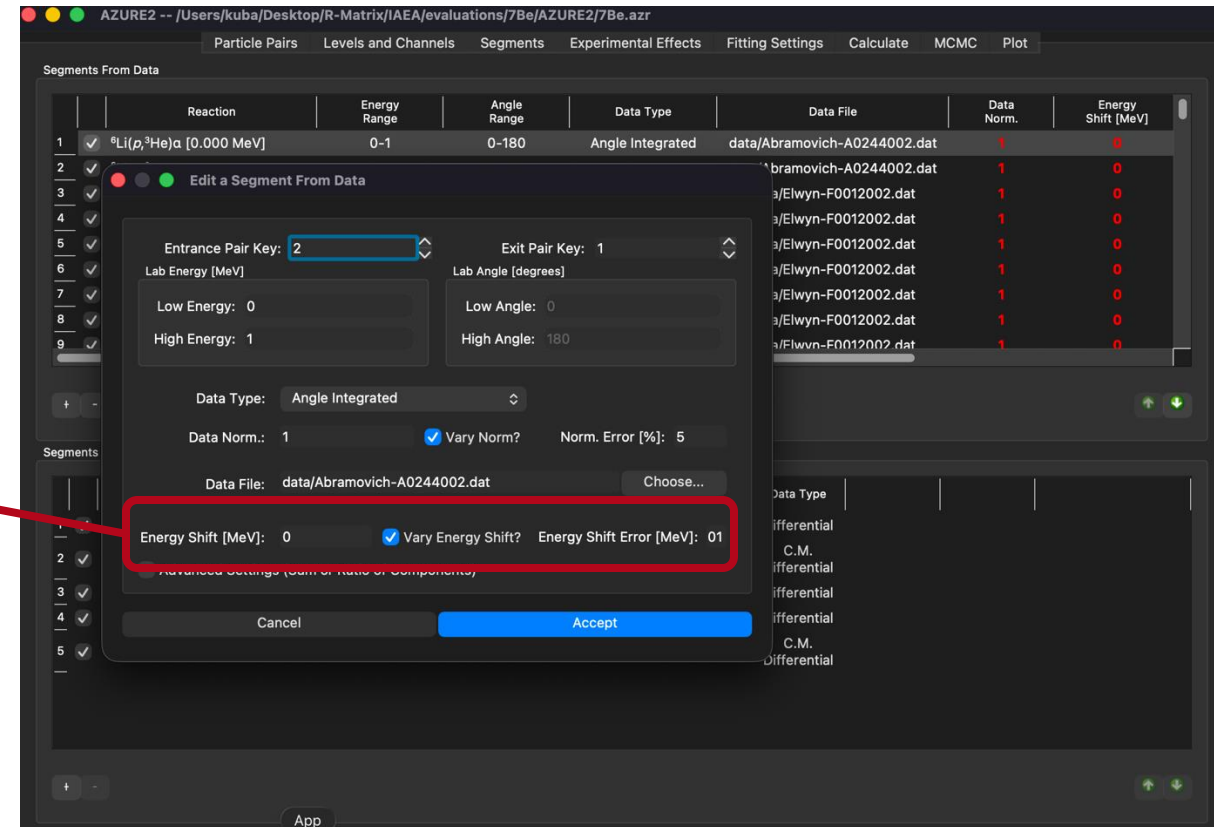
AZURE2: Energy Shifts (1)

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

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

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

New Energy Shift Term



AZURE2: Energy Shifts (1)

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

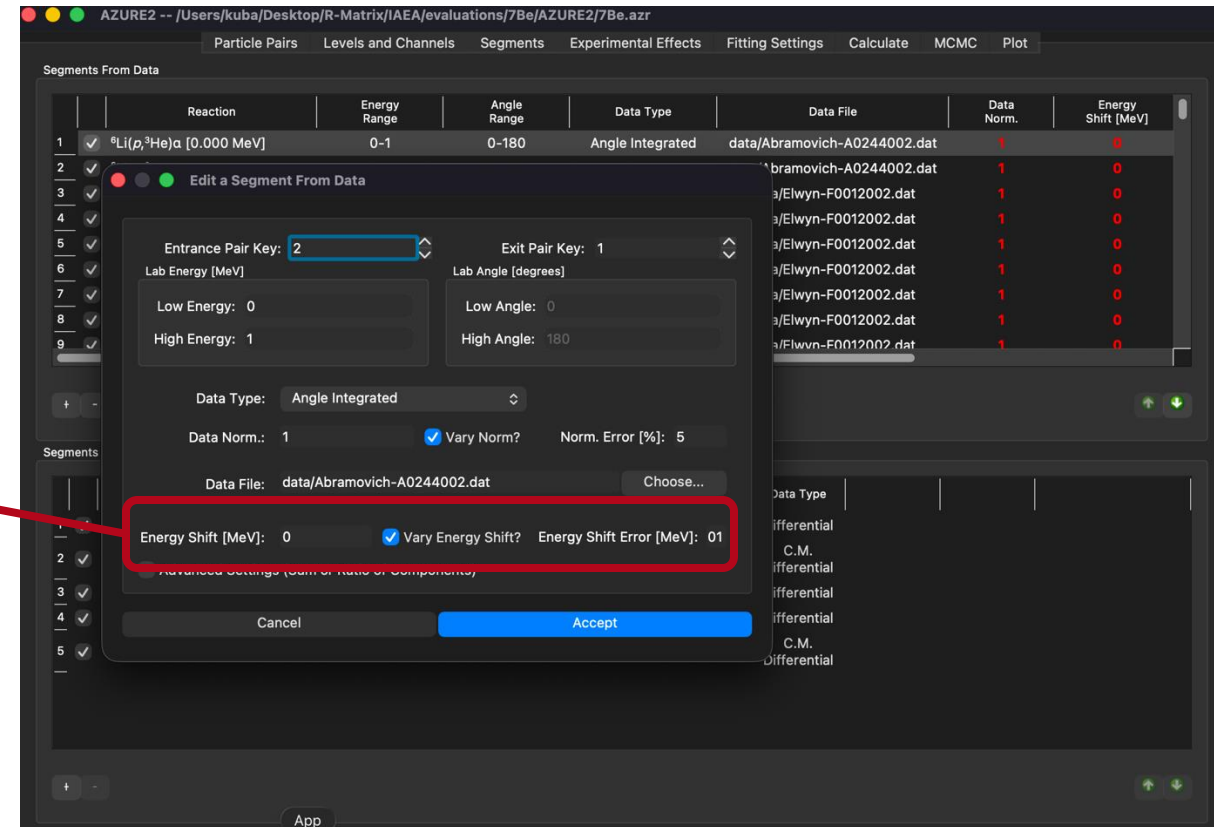
————→ **Main Impact:** underestimated uncertainties for the **resonance positions**

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

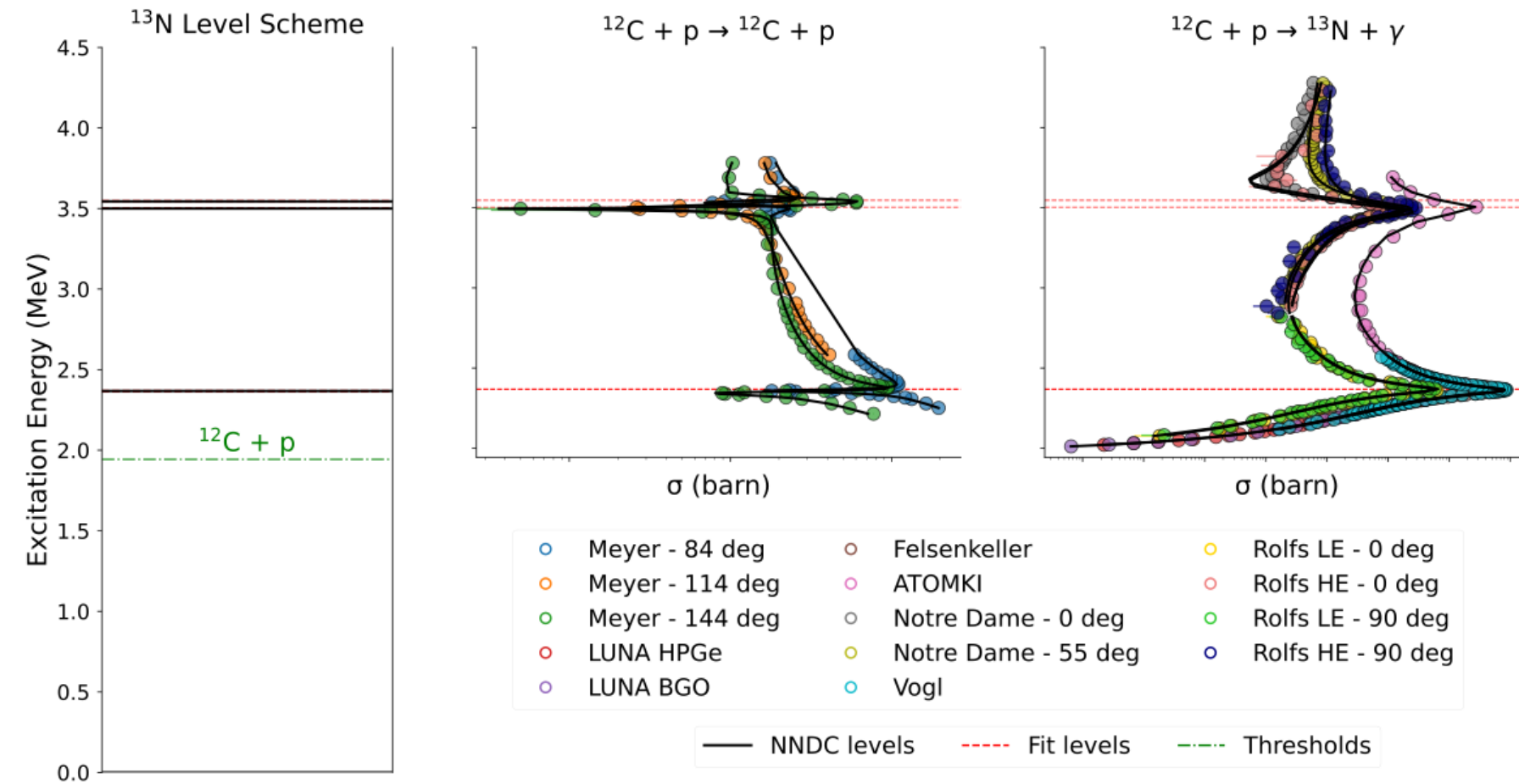
The term $\left(\frac{\Delta_j}{\Delta_{\text{sist},j}} \right)^2$ is highlighted with a red box and labeled as the **New Energy Shift Term**.

New Energy Shift Term

Quite expensive computationally
At each shift change, the code needs to recompute the coulomb wavefunctions...



AZURE2: Energy Shifts (2)

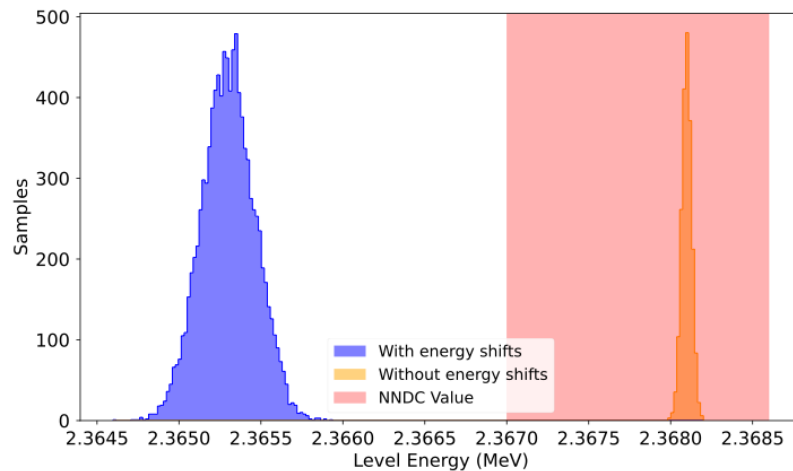


$^{12}\text{C}(p,\gamma)^{13}\text{N}$ Benchmark

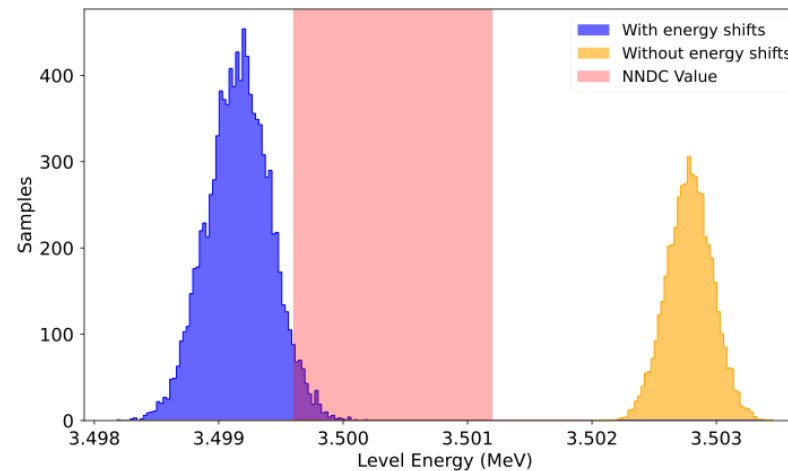
- Frequently used reaction as benchmark
- Three** different resonances
- Rolfs** dataset seems to have an **energy shift** w.r.t. to newest data
- 1 keV uncertainty** for the new measurements
- No uncertainty** for Rolfs and Vogl data

AZURE2: Energy Shifts (3)

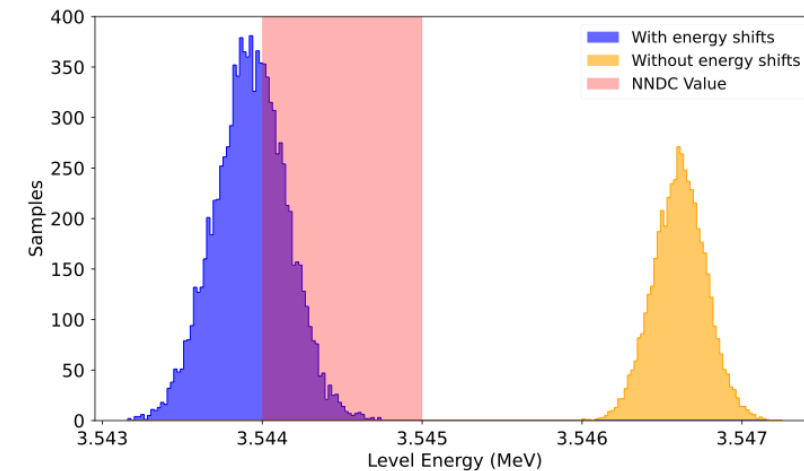
2.365 MeV State



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 now possible to define a segment with multiple input/output channels

Segments From Data

	Reaction
1	☒ $^{14}\text{N}(n,\alpha)^{11}\text{B}$ [0.000 MeV] + $^{14}\text{N}(n,n)^{14}\text{N}$ [0.000 MeV] + $^{14}\text{N}(n,p)^{14}\text{C}$ [0.000 MeV]
2	☐ $^{14}\text{N}(n,n)^{14}\text{N}$ [0.000 MeV]
3	☐ $^{14}\text{N}(n,p)^{14}\text{C}$ [0.000 MeV]
4	☒ $^{11}\text{B}(\alpha,n)^{14}\text{N}$ [0.000 MeV]
5	☒ $^{11}\text{B}(\alpha,n)^{14}\text{N}$ [0.000 MeV]

Segments Without Data

	Reaction
1	☒ $^{14}\text{N}(n,\alpha)^{11}\text{B}$ [0.000 MeV]
2	☒ $^{14}\text{N}(n,n)^{14}\text{N}$ [0.000 MeV]
3	☒ $^{14}\text{N}(n,p)^{14}\text{C}$ [0.000 MeV]
4	☐ $^{14}\text{N}(n,p)^{14}\text{C}$ [0.000 MeV]

Edit a Segment From Data

Entrance Pair Key: 2 Exit Pair Key: 1

Lab Energy [MeV] Low Energy: 0.2 High Energy: 2

Lab Angle [degrees] Low Angle: 0 High Angle: 180

Data Type: Angle Integrated

Data Norm.: 1 Vary Norm? Norm. Error [%]: 1

Data File: data/ELBE_ntot.dat Choose...

Energy Shift [MeV]: 0 Vary Energy Shift? Energy Shift Error [MeV]: 0

☒ Advanced Settings (Sum or Ratio of Components)

Advanced Segment Definition

Operation: Sum

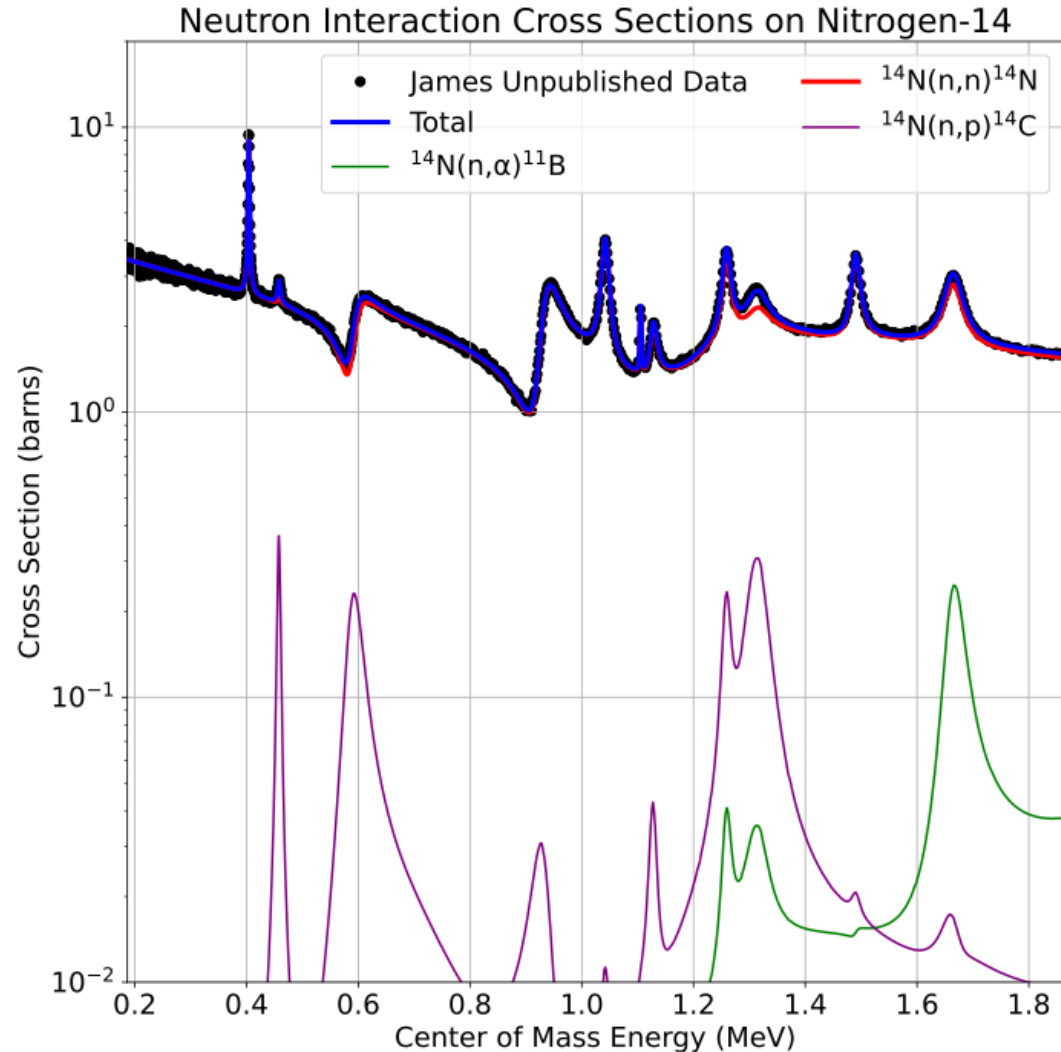
Components: Entrance: 2, Exit: 2 Entrance: 2, Exit: 3

Entrance Pair Key: 1 Exit Pair Key: 1

Add Component Remove Component

Cancel Accept

AZURE2: Reaction Channel Summing / Ratioing (2)

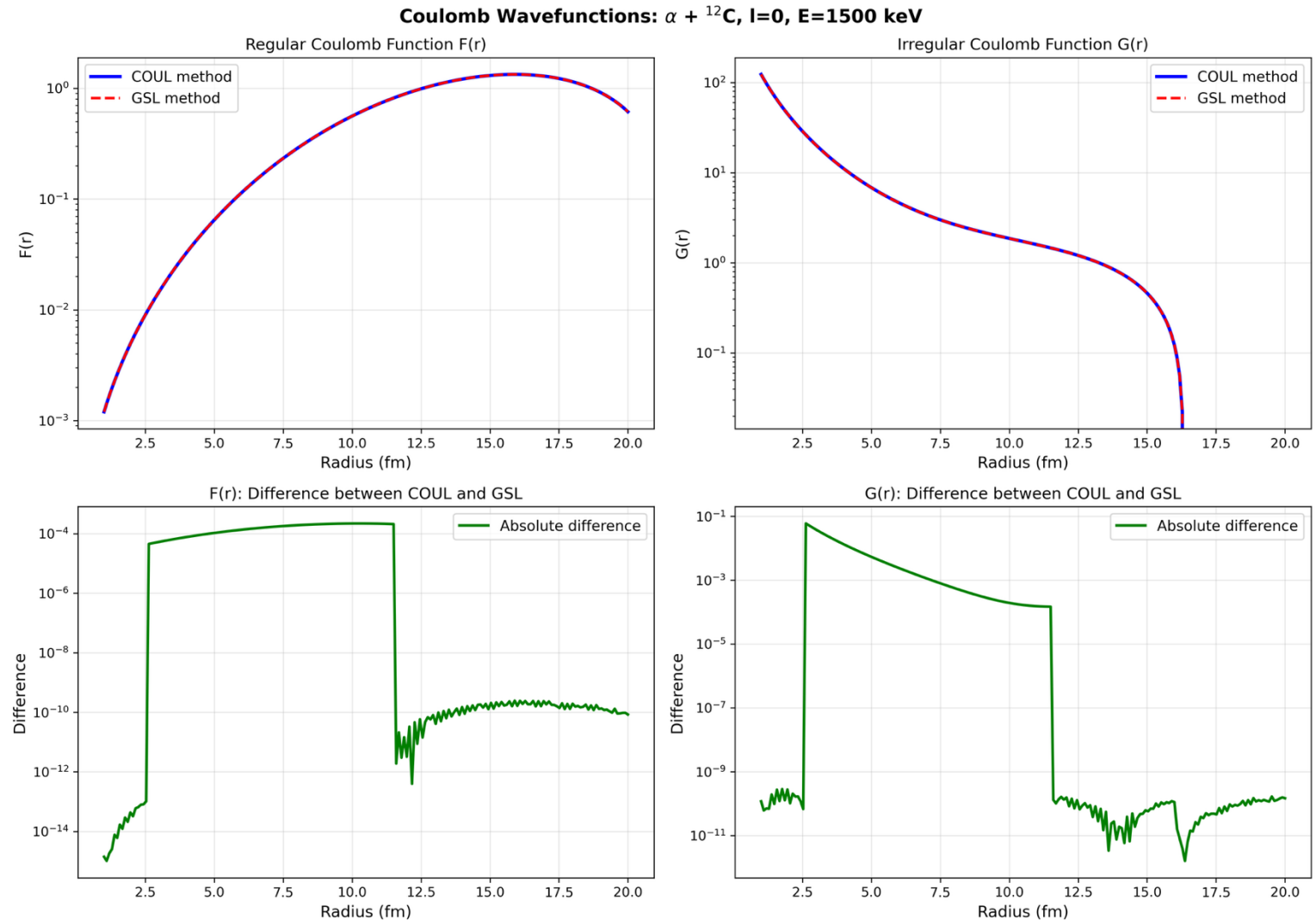


See **James's talk** for more details on the ^{15}N compound evaluation

AZURE2: Coulomb Wavefunction

Coulomb Wavefunction Improvements

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

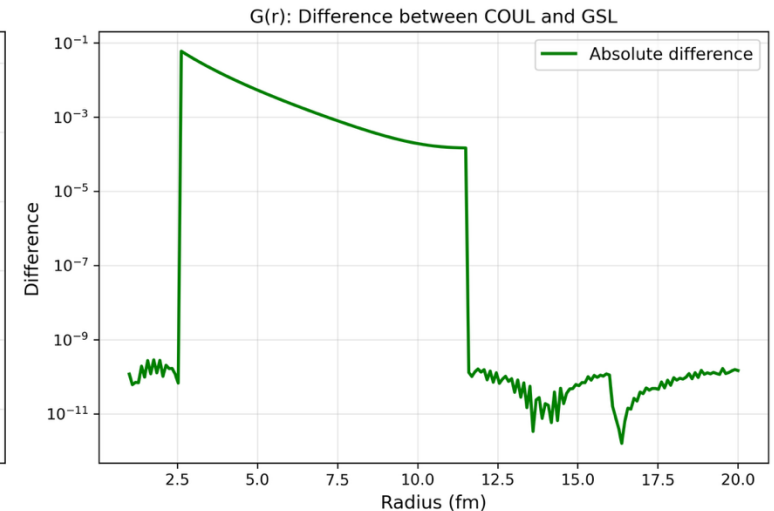
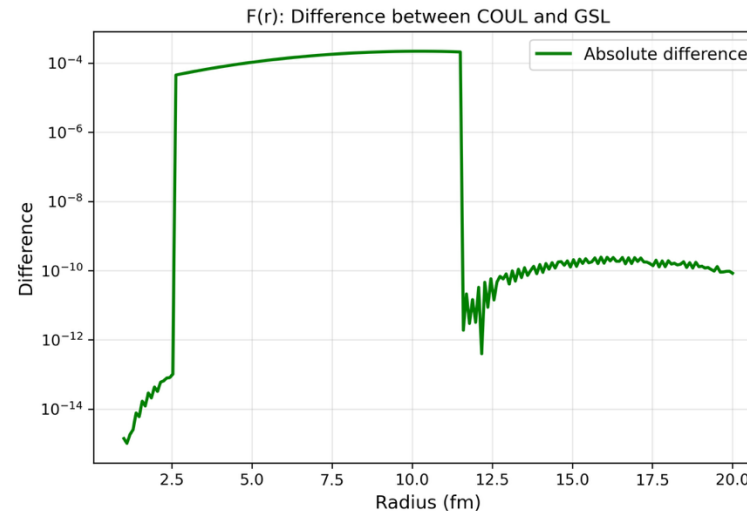
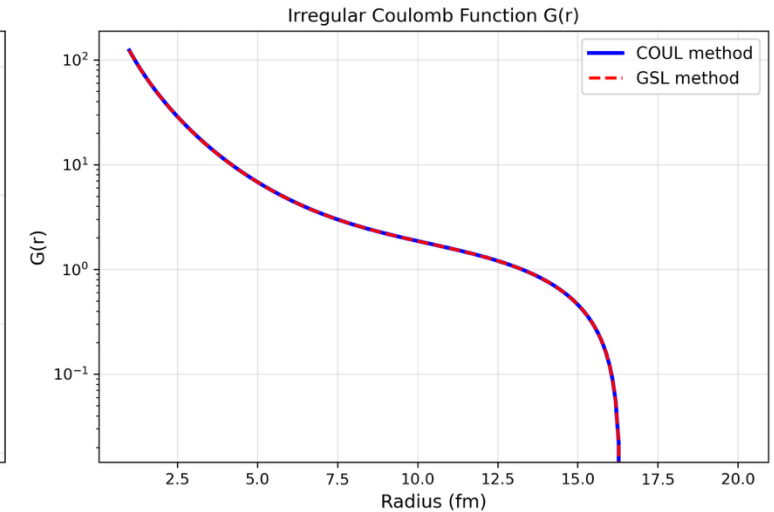
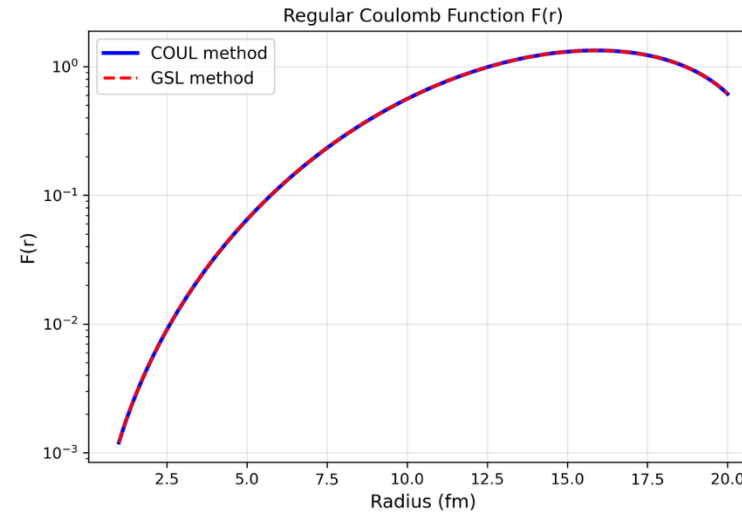


AZURE2: Coulomb Wavefunction

Coulomb Wavefunction Improvements

1. A package was created ([pycoulomb](#)) to easily test the different CW algorithms
2. The SAMMY fix was applied for COUL: when failed, it falls back to **Asymptotic Bessel Functions**

Coulomb Wavefunctions: $\alpha + {}^{12}\text{C}$, $l=0$, $E=1500$ keV



AZURE2: Coulomb Wavefunction

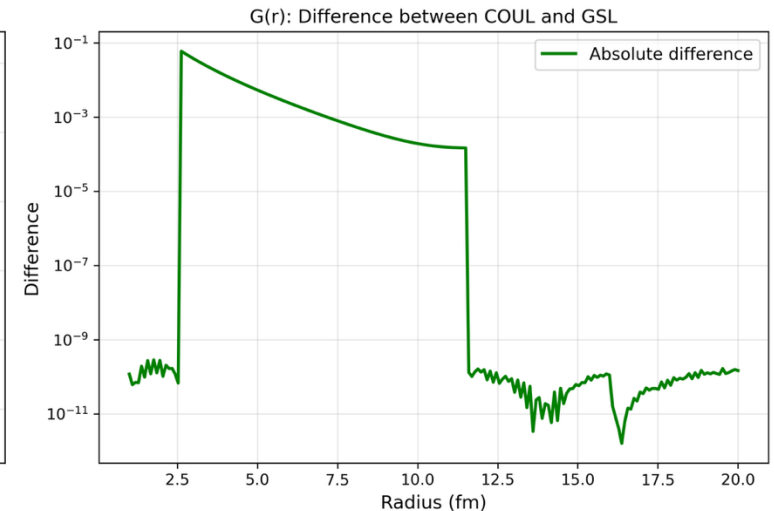
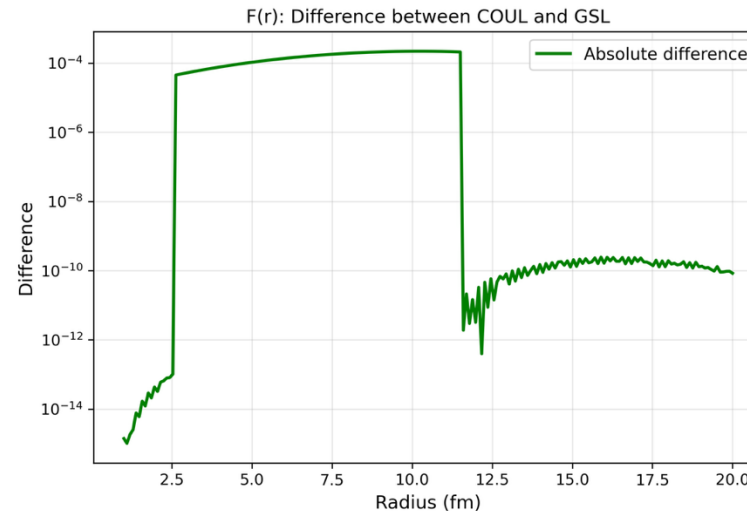
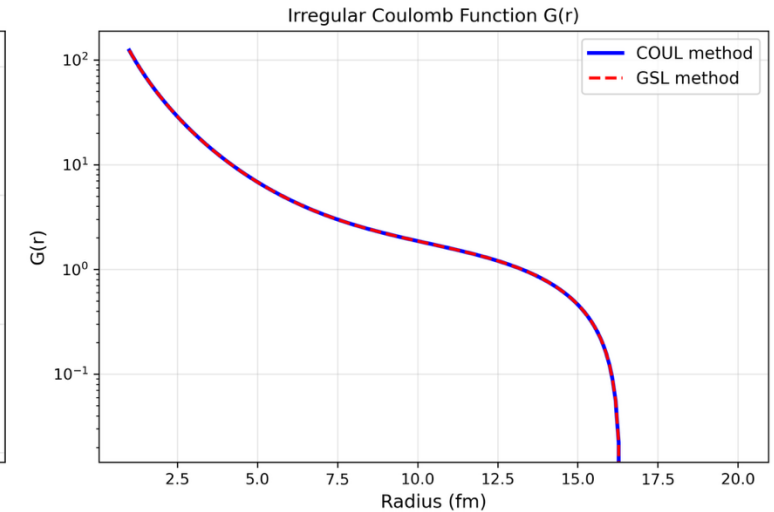
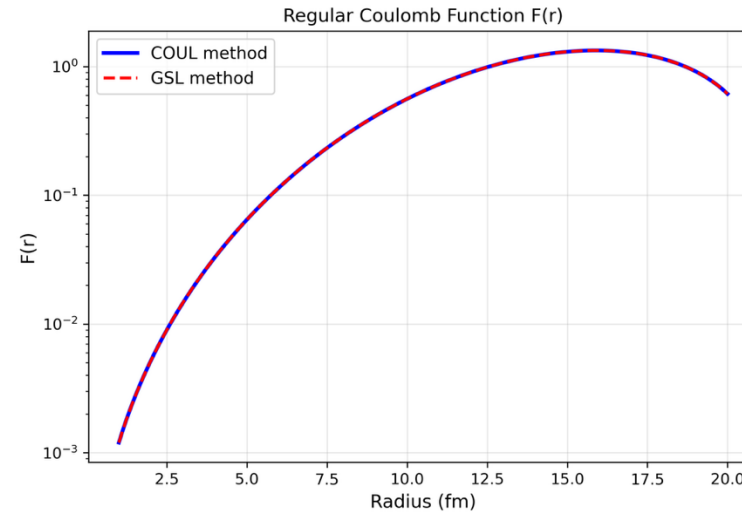
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↓
**No more AZURE2
crashes**

↓
**Extrapolations
down to 1 eV**

Coulomb Wavefunctions: $\alpha + {}^{12}\text{C}$, $l=0$, $E=1500$ keV



AZURE2: Coulomb Wavefunction

Coulomb Wavefunction Improvements

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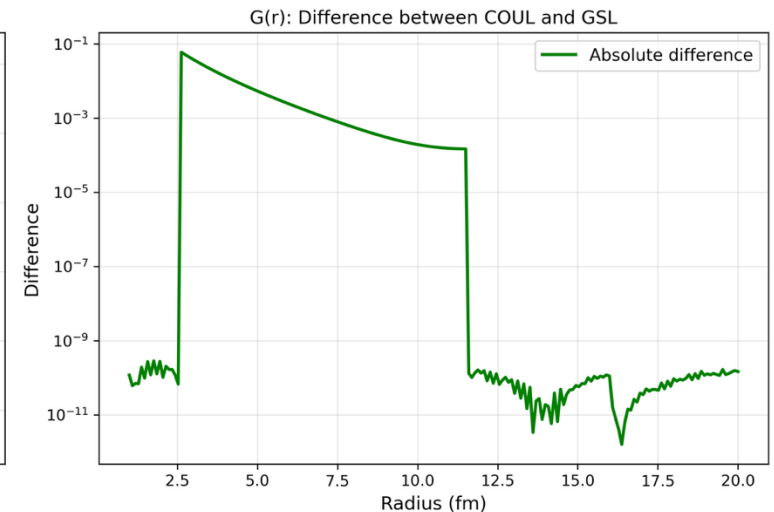
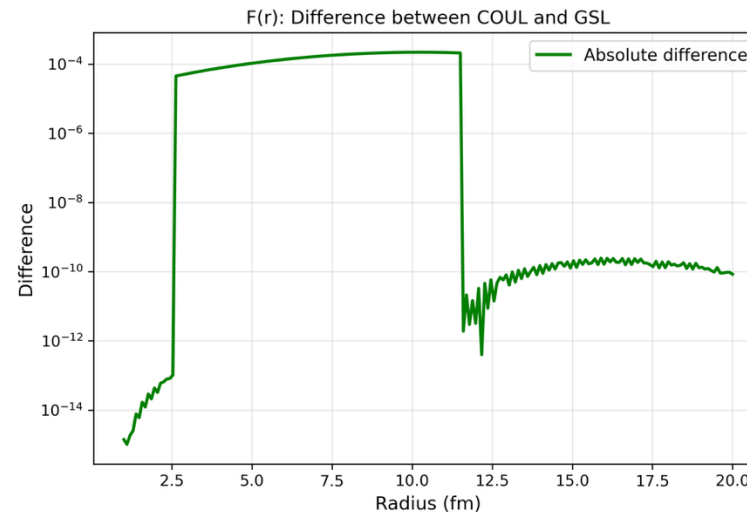
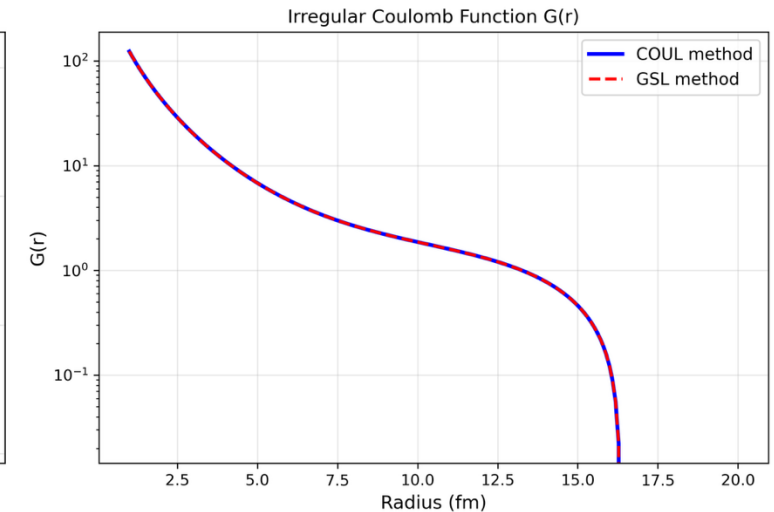
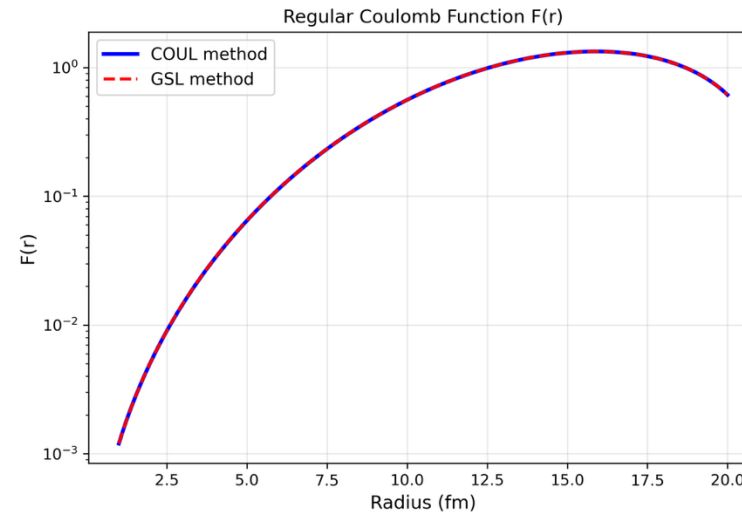
↓
**No more AZURE2
crashes**

↓
**Extrapolations
down to 1 eV**

+

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

Coulomb Wavefunctions: $\alpha + {}^{12}\text{C}$, $l=0$, $E=1500$ keV



AZURE2: Infinite Target Yield (1)

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

Edit an Experimental Effect Line

Segments List: Number of Integration Points: 10

☐ Include Gaussian Convolution Sigma [MeV]: 0

☒ Include Target Integration Active Density [atoms/cm^2]: 0

Energy [keV]: 1000.0 ΔE [keV]: Calculate ΔE

Effective Stopping Cross Section [MeV cm^2/atoms]

Target Element:

Or Compound Formula: Fetch from ERYA

☐ Include Energy Straggling

$y = a4 / ((x \cdot 1e3)^{a5} \cdot \ln(a6 / (x \cdot 1e3) + a7 \cdot (x \cdot 1e3))) + (a0 \cdot (x \cdot 1e3)^{a1} + a2 \cdot (x \cdot 1e3)^{a3}) / 1e+21$ Number of Parameters: 8

Parameter	Value
a0	2.402890
a1	0.00491497

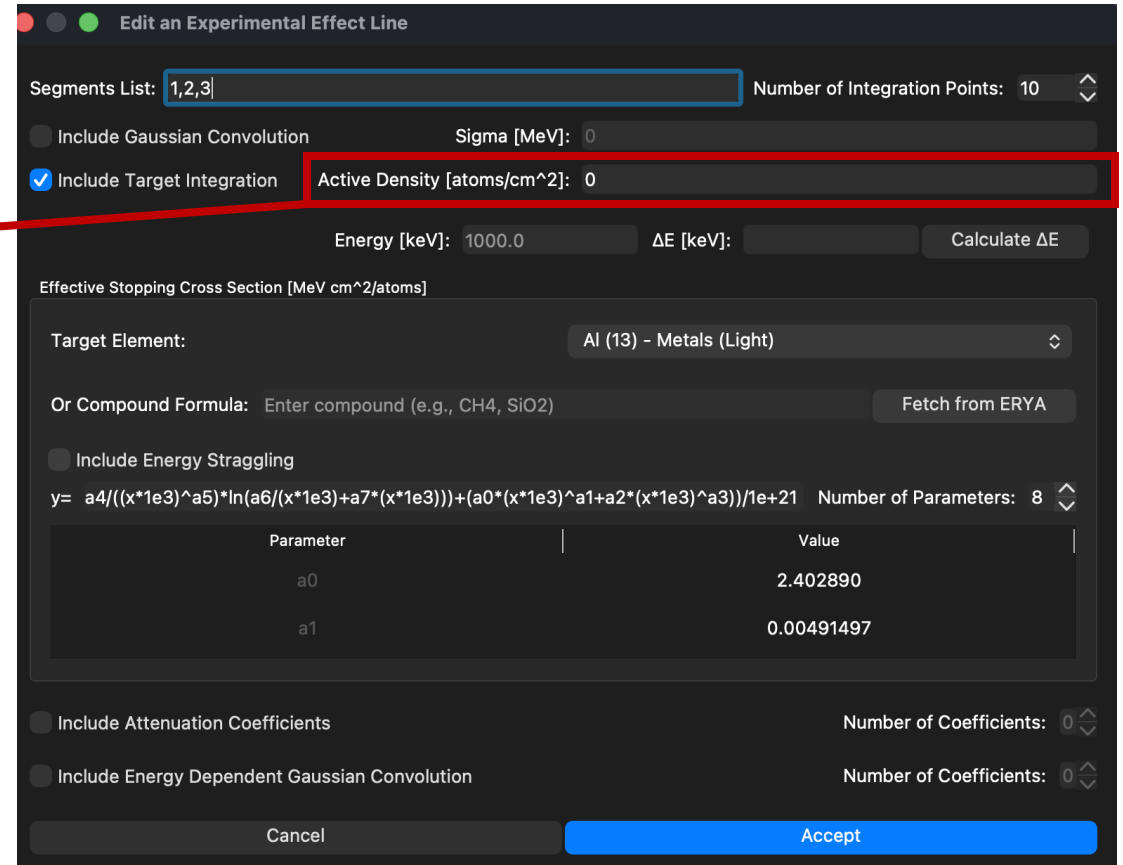
☐ Include Attenuation Coefficients Number of Coefficients: 0

☐ Include Energy Dependent Gaussian Convolution Number of Coefficients: 0

AZURE2: Infinite Target Yield (1)

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

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



Edit an Experimental Effect Line

Segments List: 1,2,3 | Number of Integration Points: 10

☐ Include Gaussian Convolution | Sigma [MeV]: 0

☒ Include Target Integration | **Active Density [atoms/cm^2]: 0**

Energy [keV]: 1000.0 | ΔE [keV]: | Calculate ΔE

Effective Stopping Cross Section [MeV cm^2/atoms]

Target Element: Al (13) - Metals (Light)

Or Compound Formula: Enter compound (e.g., CH4, SiO2) | Fetch from ERYA

☐ Include Energy Straggling

$y = a4 / ((x \cdot 1e3)^{a5} \cdot \ln(a6 / (x \cdot 1e3) + a7 \cdot (x \cdot 1e3))) + (a0 \cdot (x \cdot 1e3)^{a1} + a2 \cdot (x \cdot 1e3)^{a3}) / 1e+21$ | Number of Parameters: 8

Parameter	Value
a0	2.402890
a1	0.00491497

☐ Include Attenuation Coefficients | Number of Coefficients: 0

☐ Include Energy Dependent Gaussian Convolution | Number of Coefficients: 0

Cancel | Accept

AZURE2: Infinite Target Yield (1)

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

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

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

Dialog box titled "Edit an Experimental Effect Line".

Segments List: Number of Integration Points: 10

☐ Include Gaussian Convolution Sigma [MeV]: 0

☒ Include Target Integration Active Density [atoms/cm²]: 0

Energy [keV]: 1000.0 ΔE [keV]: Calculate ΔE

Effective Stopping Cross Section [MeV cm²/atoms]

Target Element:

Or Compound Formula:

☐ Include Energy Straggling

Equation: $y = a_4 / ((x \cdot 10^3)^{a_5} \cdot \ln(a_6 / ((x \cdot 10^3)^{a_7} + a_8))) + (a_0 \cdot (x \cdot 10^3)^{a_1} + a_2 \cdot (x \cdot 10^3)^{a_3}) / 1e+21$ Number of Parameters: 8

Parameter	Value
a0	2.402890
a1	0.00491497

☐ Include Attenuation Coefficients Number of Coefficients: 0

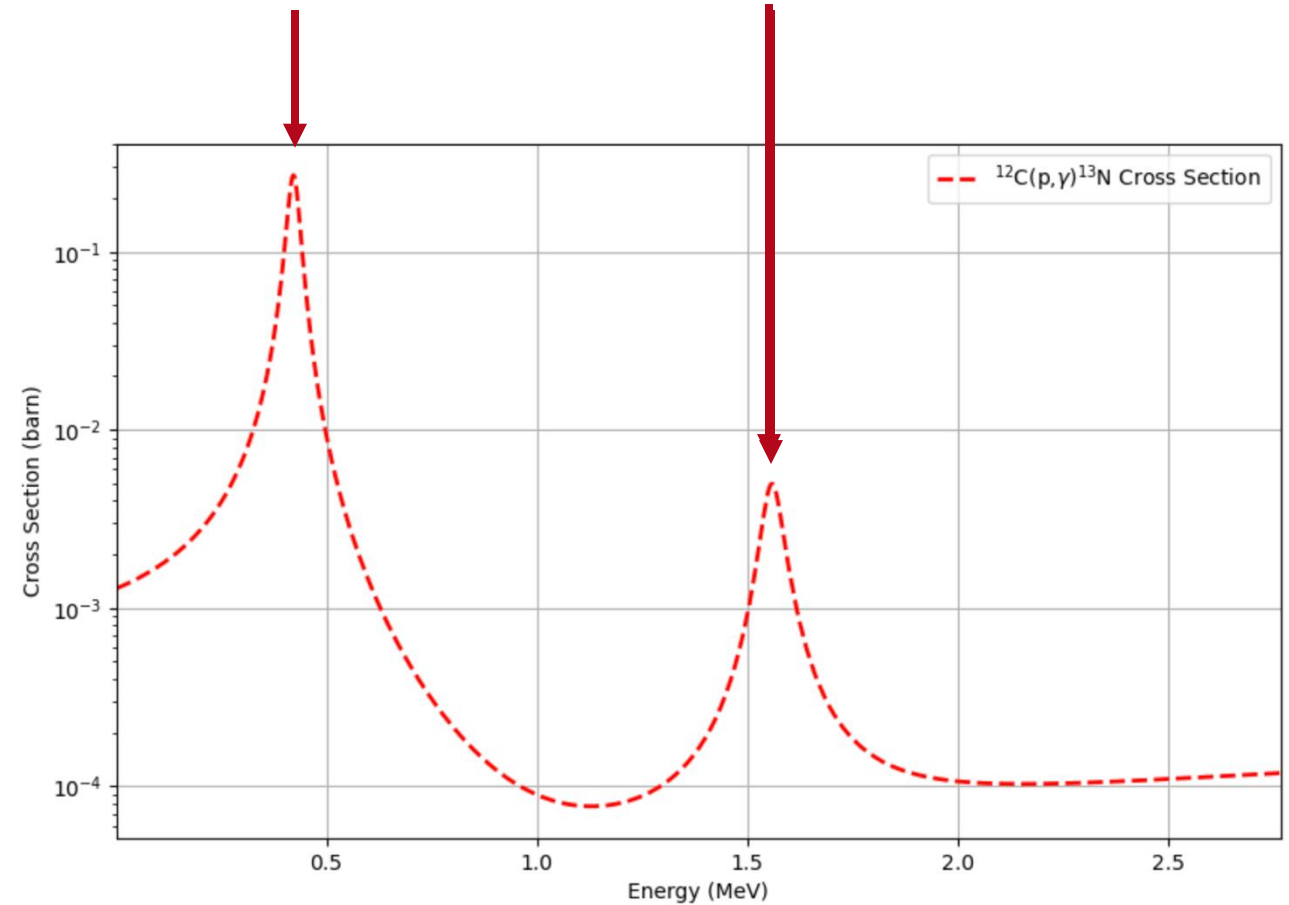
☐ Include Energy Dependent Gaussian Convolution Number of Coefficients: 0

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

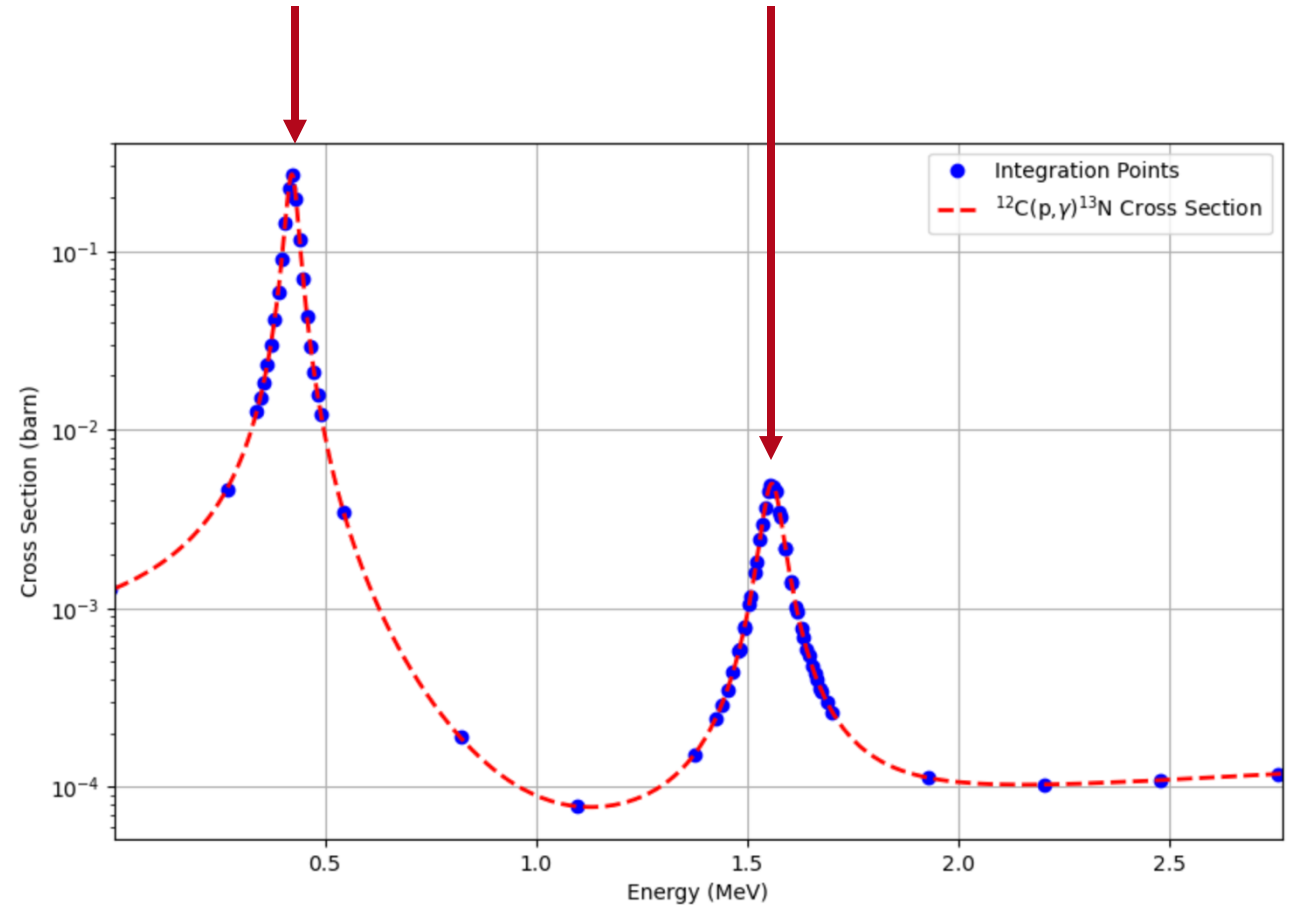


AZURE2: Infinite Target Yield (1)

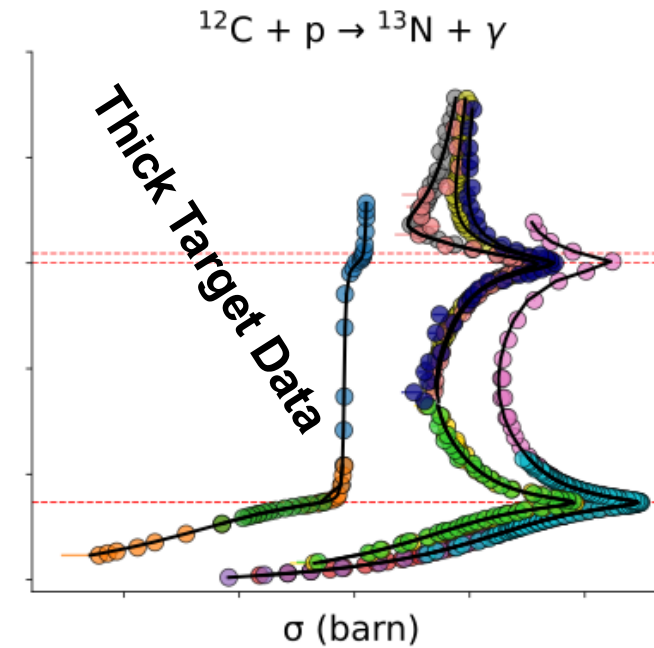
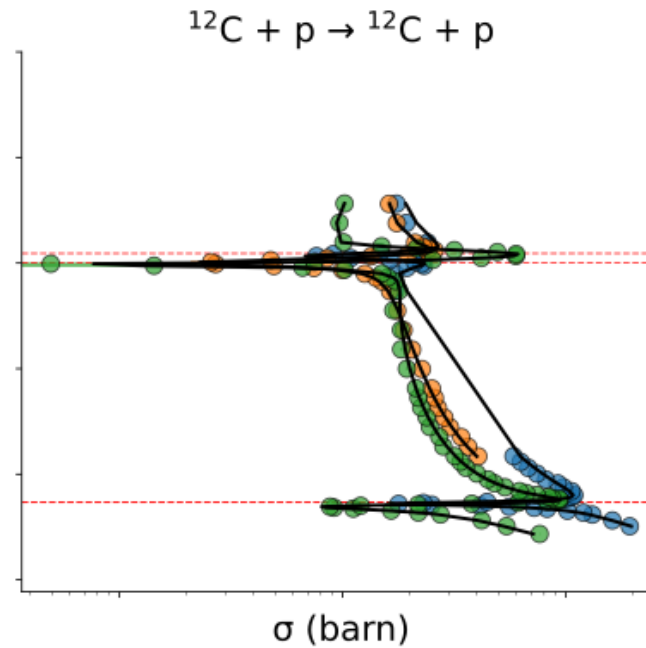
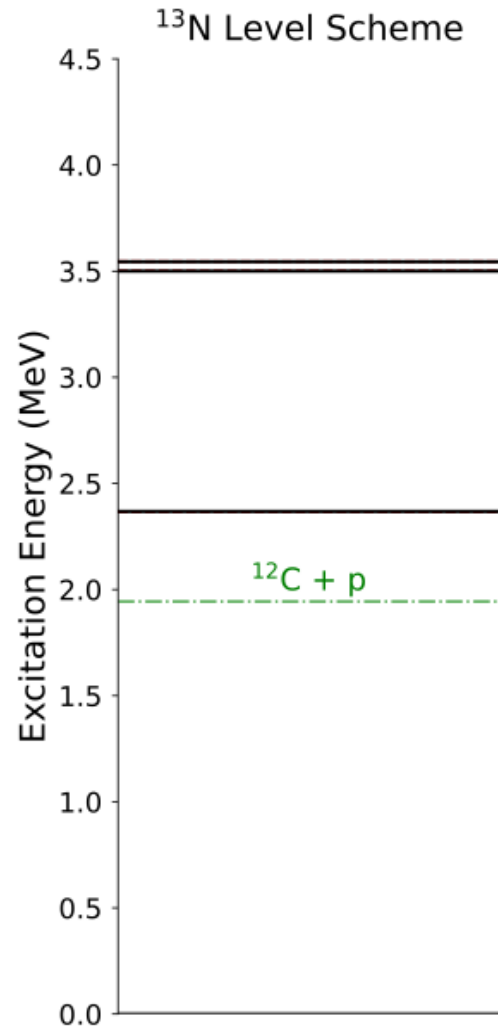
AZURE2 is now capable to calculate the **infinitely thick target yield**

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**



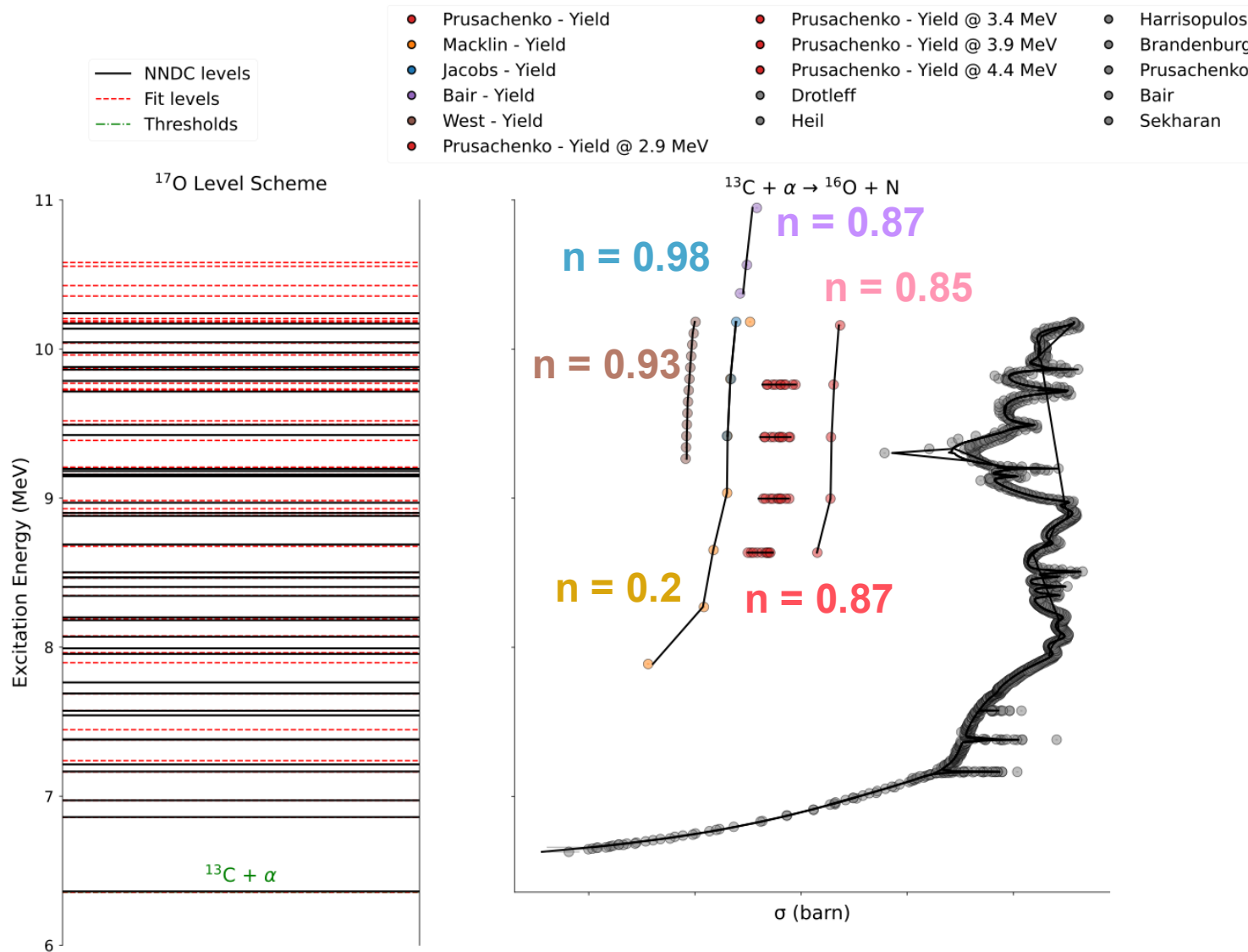
AZURE2: Infinite Target Yield (2)



— NNDC levels - - - - Fit levels - - - - Thresholds

**Agrees well
with the new
data!**

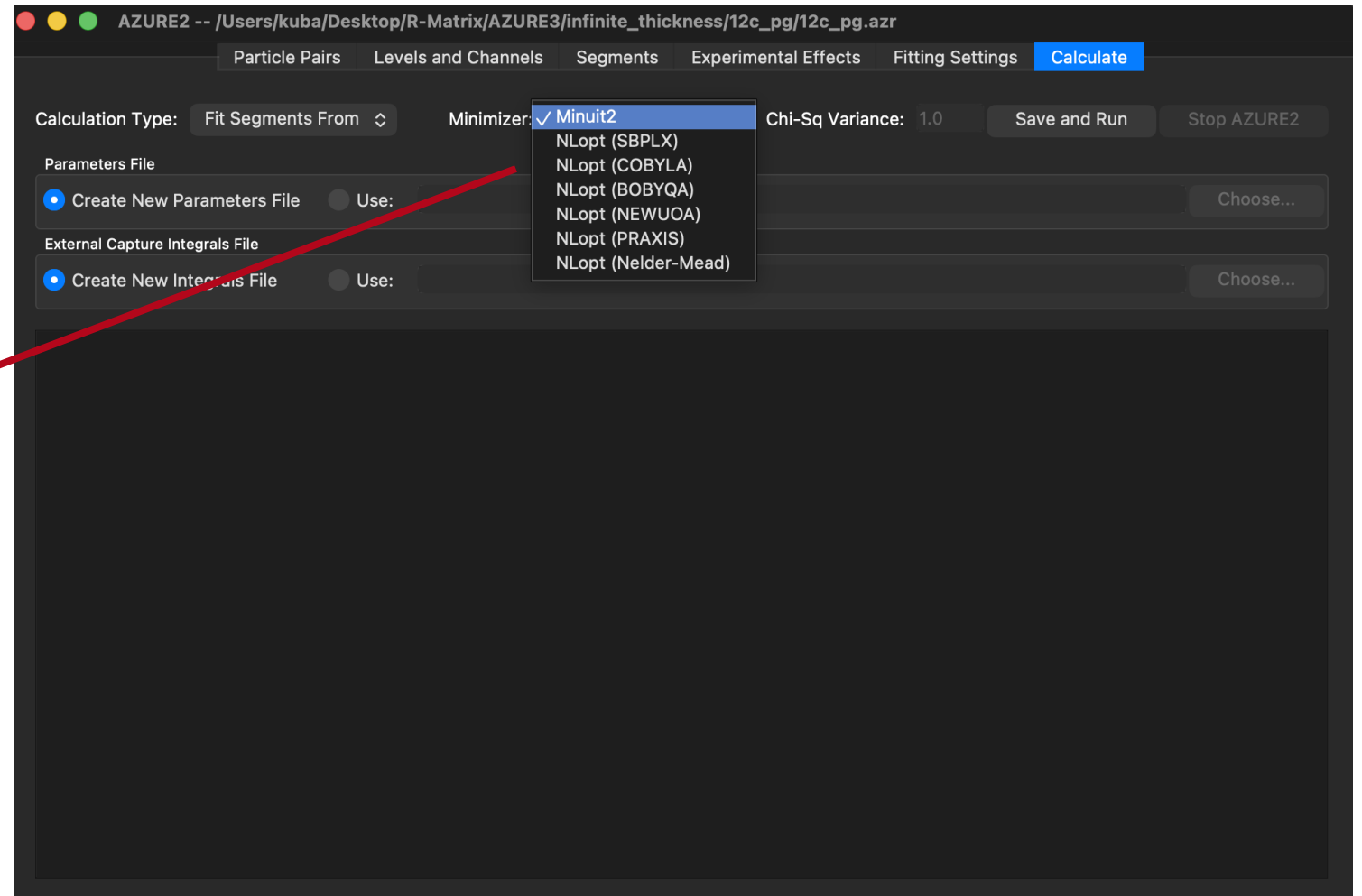
AZURE2: Infinite Target Yield (3)



- 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](https://zenodo.org/record/5496329))
was added for a native MCMC
sampling



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

The screenshot shows the AZURE2 software interface with the title bar: "AZURE2 -- /Users/kuba/Desktop/R-Matrix/AZURE3/infinite_thickness/12c_pg/12c_pg.azr". The top menu bar includes "Particle Pairs", "Levels and Channels", "Segments", "Experimental Effects", "Fitting Settings", "Calculate", "MCMC", and "Plot". The "MCMC" tab is active, showing sub-tabs for "Parameters", "Sampling Settings", and "Results".

The "Parameters" sub-tab displays a table with the following data:

	Parameter	Current Value	Prior Mean	Prior Std	Use Gaussian Prior	Category
1	Parameter ...	1.62	1.62	0.162	☐	level
2	Parameter ...	2.3682	2.3682	0.23682	☐	level
3	Parameter ...	34000	34000	3400	☐	level
4	Parameter ...	-0.48	-0.48	0.048	☐	level
5	Parameter ...	5400	5400	540	☐	level

Below the table are buttons for "Load Physical Parameters" and "Load RWA Parameters".

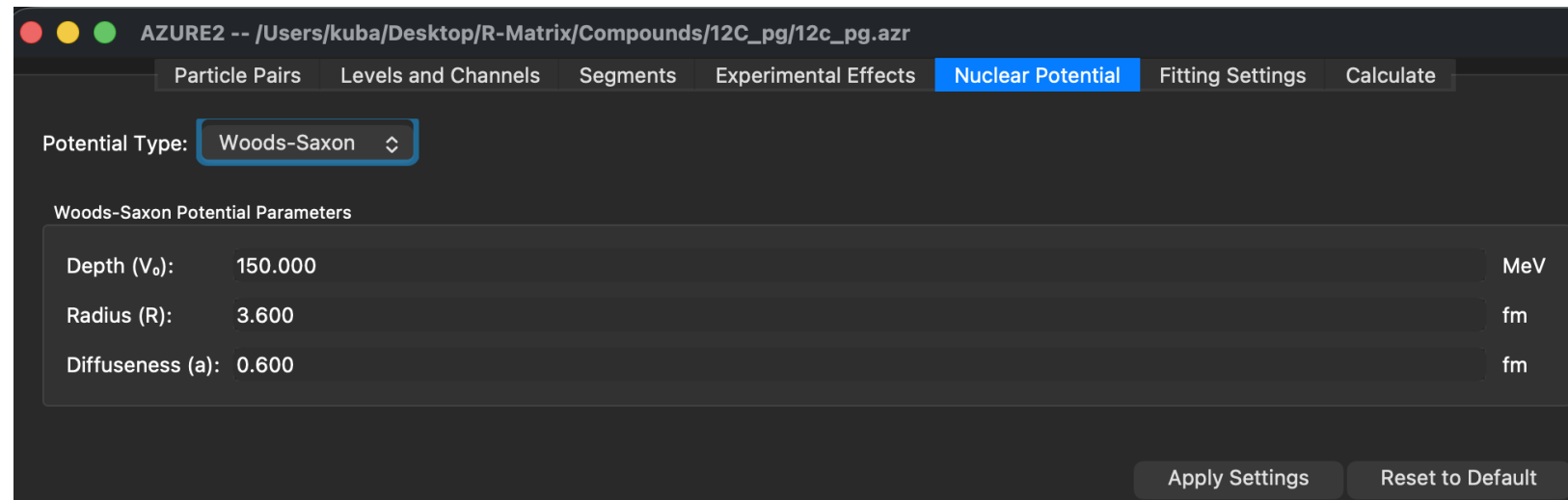
The "MCMC Control" section contains buttons for "Run MCMC Sampling", "Stop Sampling", "Fresh Start", and "Use Reduced Widths". It also displays the status: "Ready to run MCMC sampling", "Current Iteration: 0", and "Current Log Probability: N/A Log Likelihood: N/A Log Prior: N/A".

A "Sampling Log" section at the bottom shows an error message: "Error: Could not initialize compound nucleus from current configuration. Loaded MCMC settings with 0 parameters. Loaded 47 non-fixed parameters from current AZUREParams (RWA mode)".

AZURE2: (Experimental) Hybrid Potential Model

Hybrid Potential Model was implemented in AZURE2

1. Coulomb Wavefunction is calculated at $r = 15 \text{ fm}$ 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

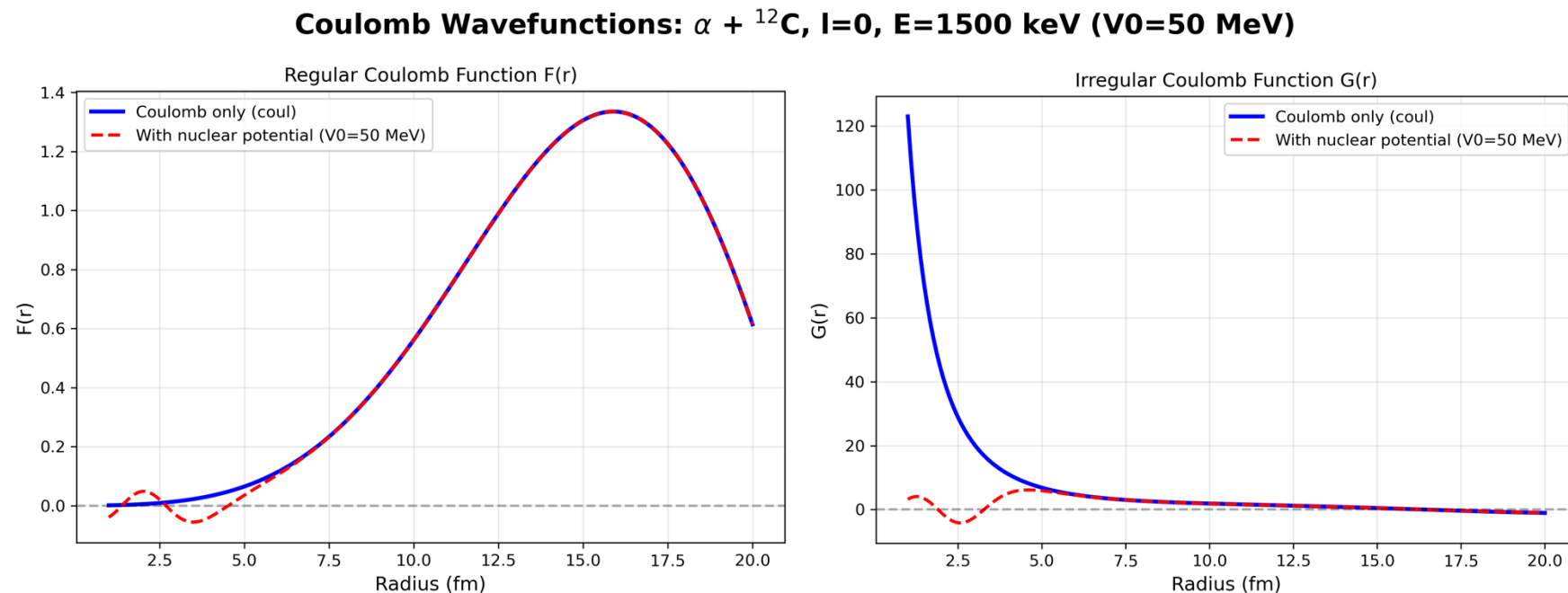


AZURE2: (Experimental) Hybrid Potential Model

Hybrid Potential Model was implemented in AZURE2

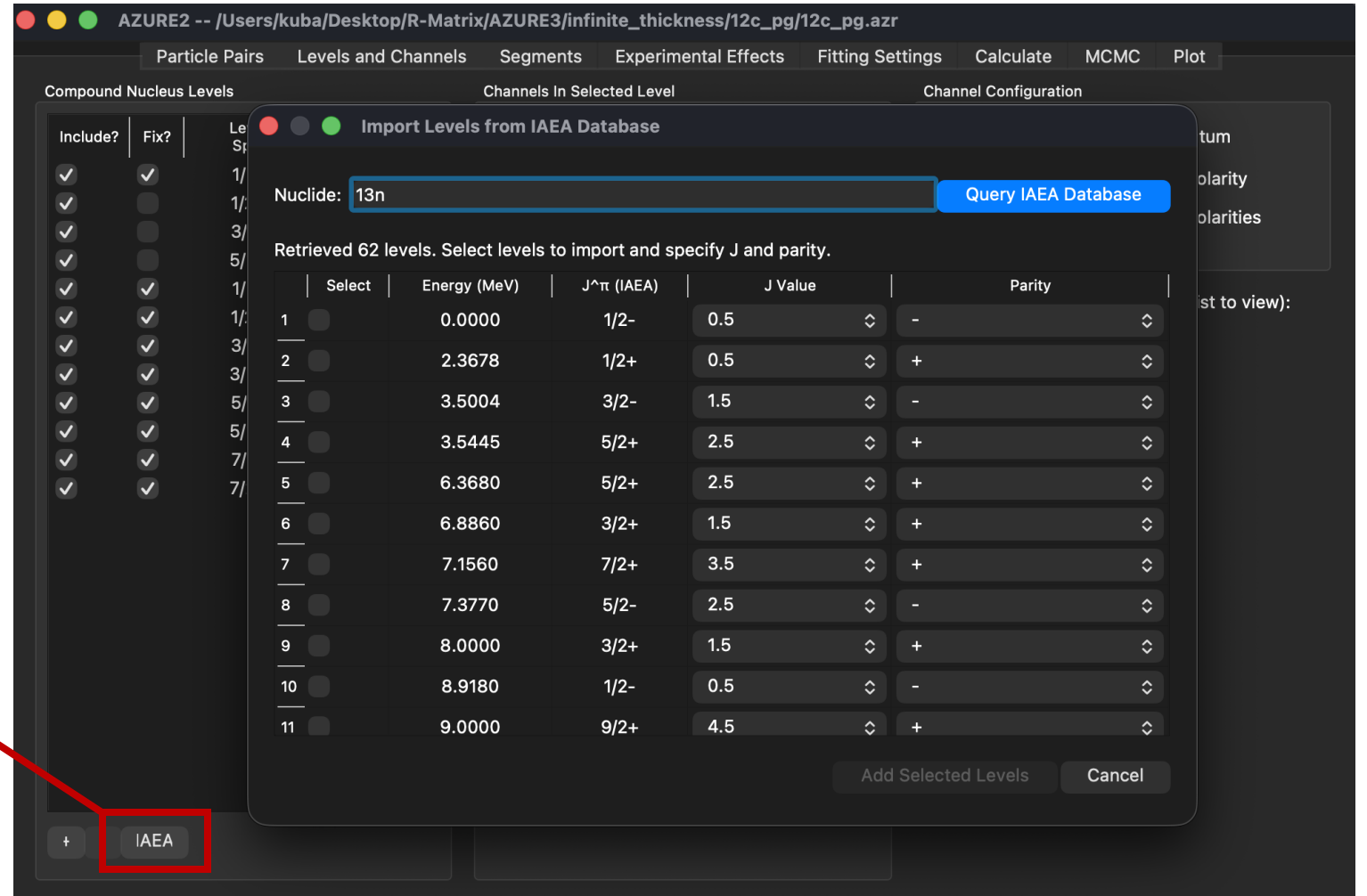
1. Coulomb Wavefunction is calculated at $r = 15 \text{ fm}$ with COUL algorithm
2. Then the wavefunction is obtained at the desired radius by using the **Numerov integration method**
3. During the integration, a **Woods-Saxon + Coulomb** potential is assumed with V_0 , a_s and r_s

- 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>

AZURE2 Compounds Data Levels Data Plotter Extrapolation Plotter Fitting

Compounds

Select a compound nucleus to show its evaluation

✓ ⁷Be loaded

📄 ¹³N

Reference: 10.1103/PhysRevC.111.035802
Author: J. Skowronski

Select Project

📄 ¹⁴N

Reference: 10.1103/h1yt-5myk
Author: J. Skowronski

Select Project

📄 ²¹Na

Reference: 10.1103/PhysRevC.108.L052801
Author: J. Skowronski

Select Project

📄 ⁷Be

Reference: Unpublished
Author: R. J. deBoer & J. Skowronski

Selected

App

^7Be Compound Evaluation

⁷Be Evaluation with AZURE2

Channels

³He + ⁴He

⁶Li + p

Separation Energy

1.58649 MeV

5.6063 MeV

Channel Radius

4.24151 fm

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)

⁷Be Evaluation with AZURE2

Channels

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Tumino (O1221002)

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

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

⁷Be Evaluation with AZURE2

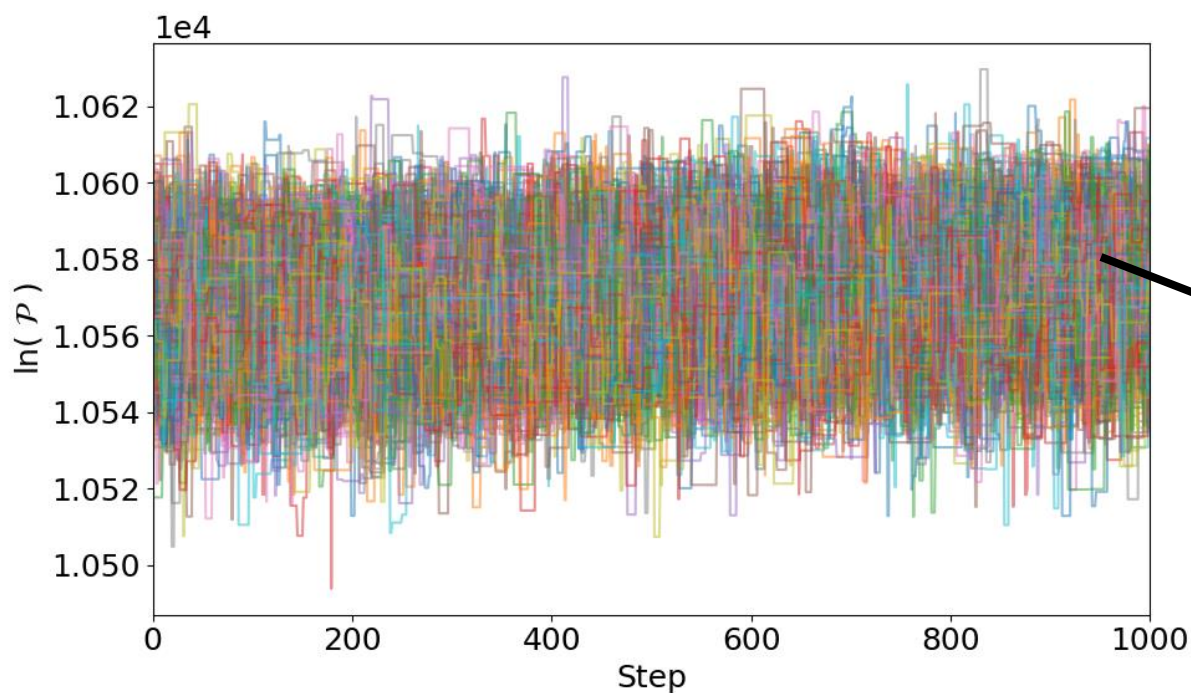
- Best **frequentist fit** reached reduced $\chi^2 = 1.8$
- Covariance matrix calculation **failed**

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⁷Be 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

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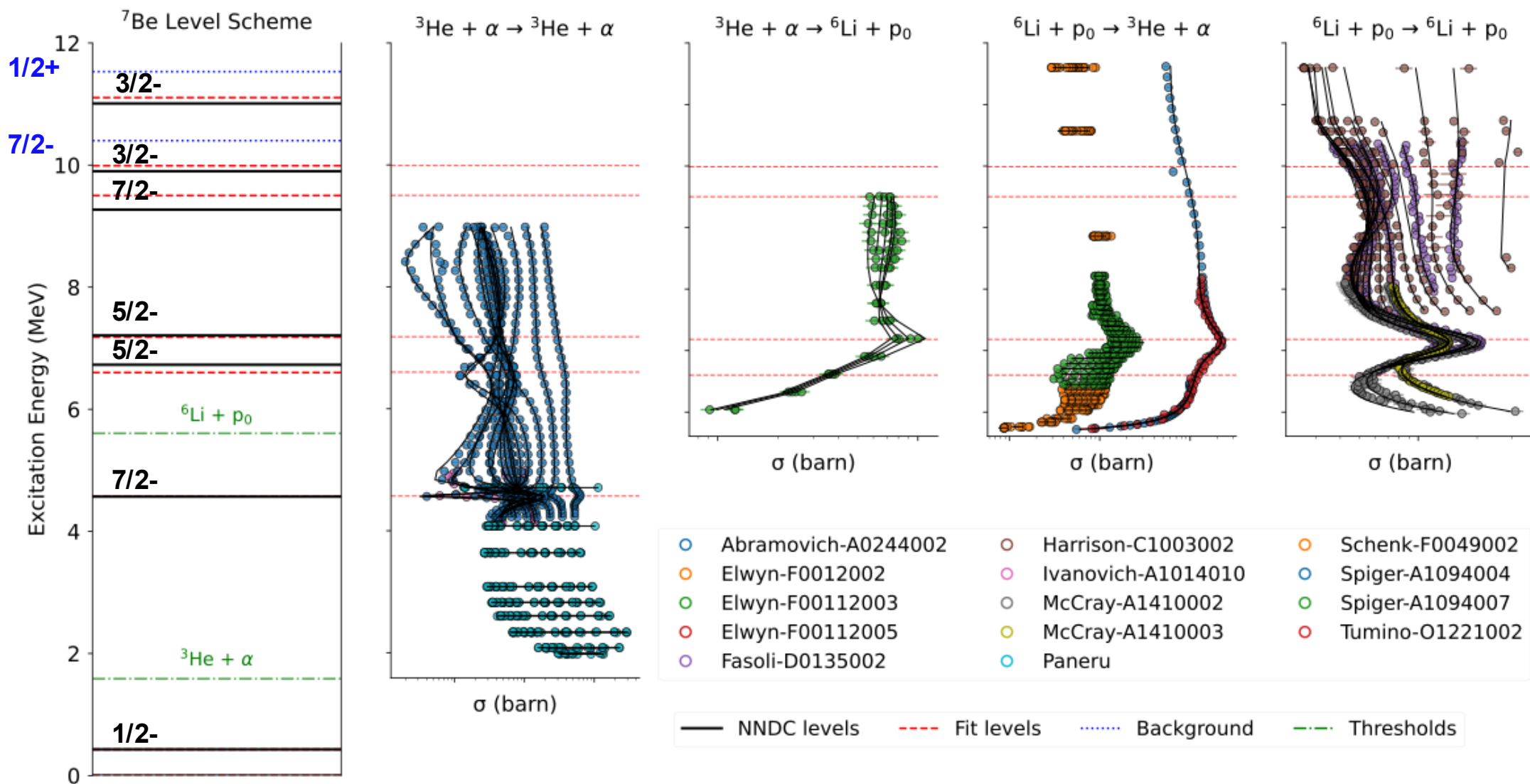
Paneru

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Spiger (A1094004/7)

Tumino (O1221002)

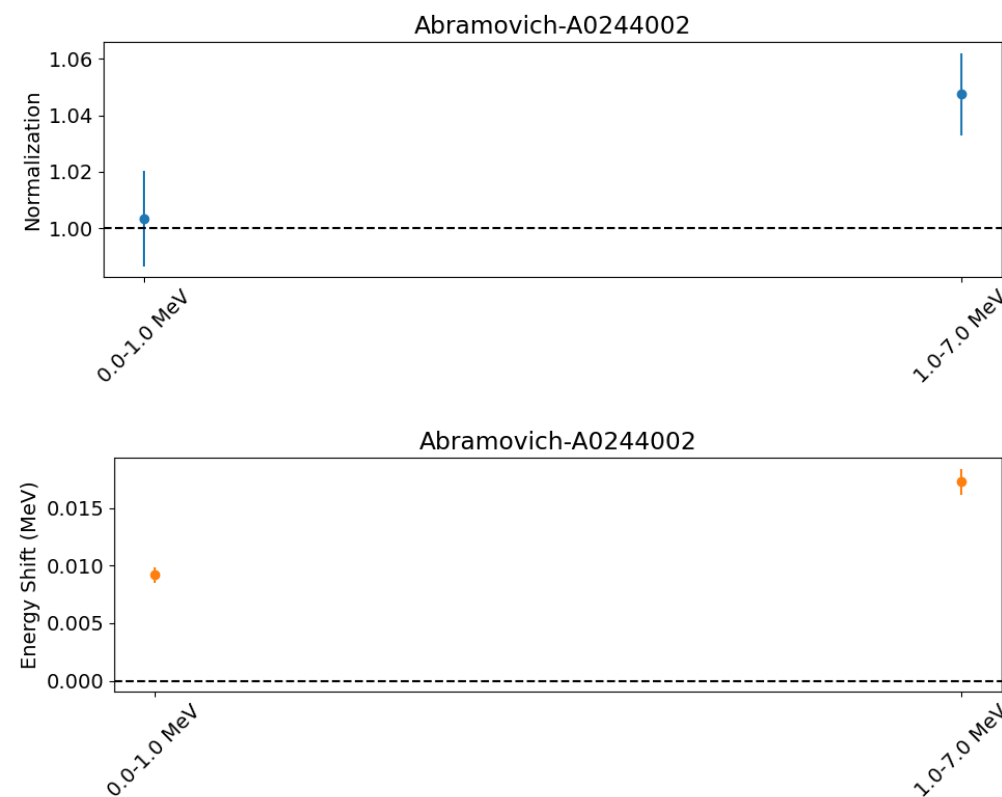
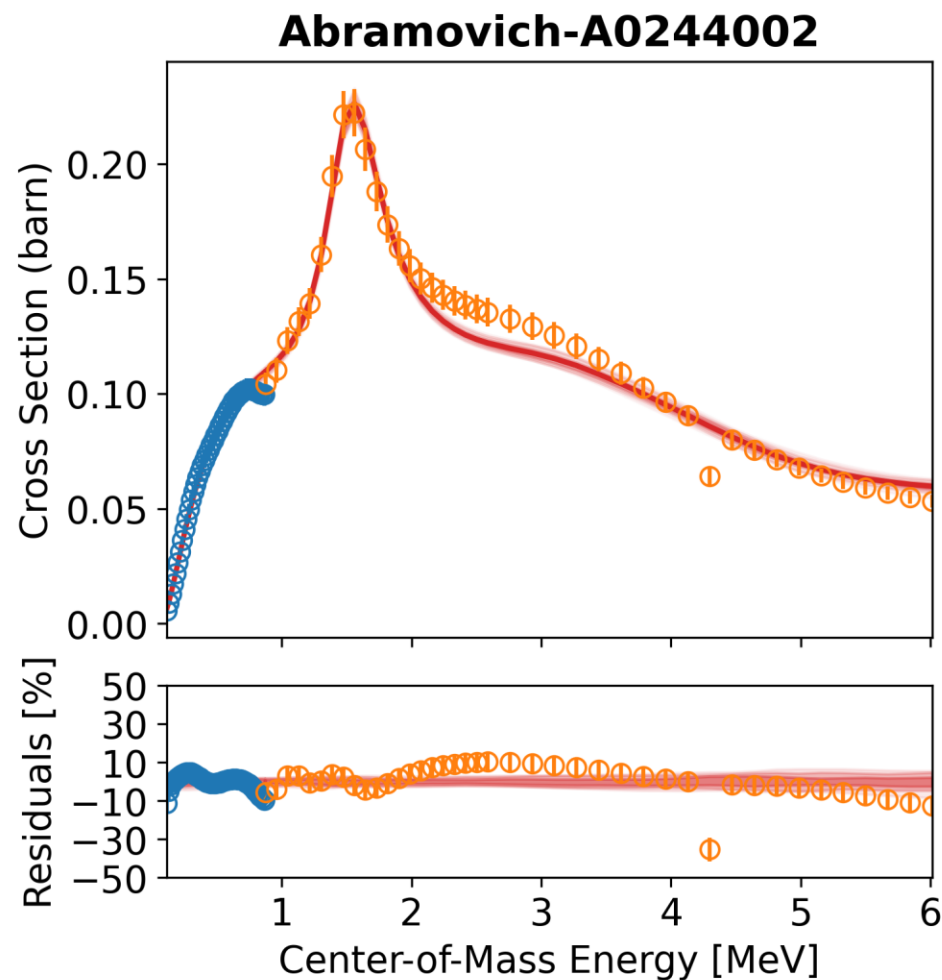
^7Be Evaluation with AZURE2: Result



^7Be Evaluation with AZURE2: Segments

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^7Be Evaluation with AZURE2: Segments

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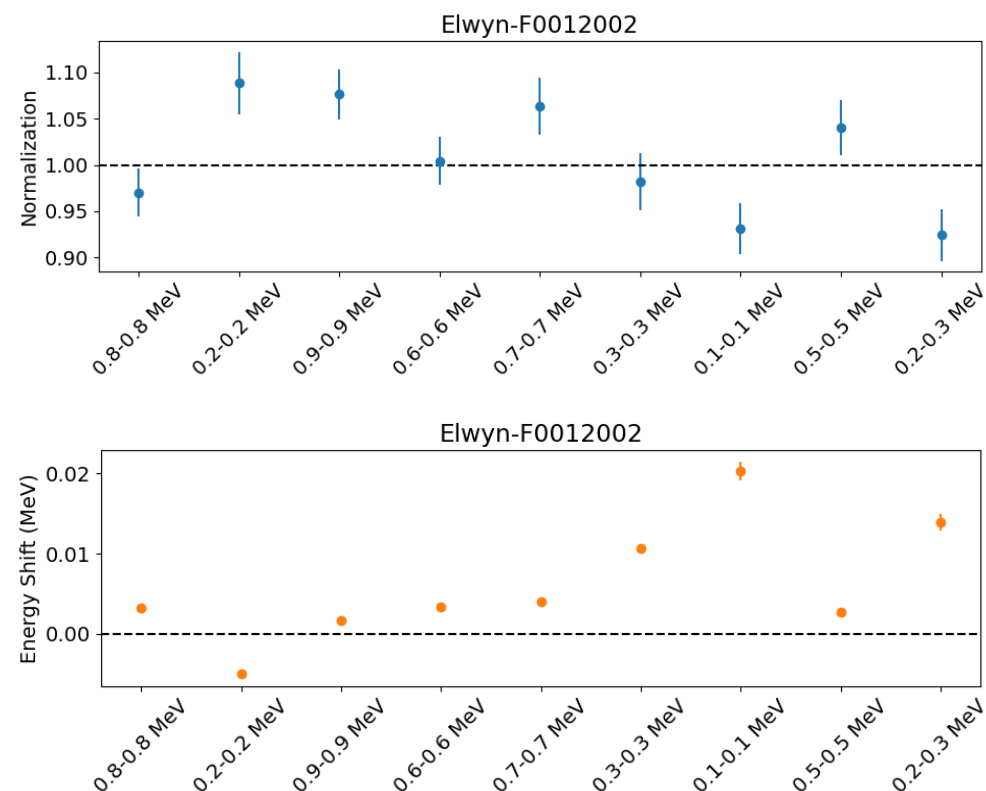
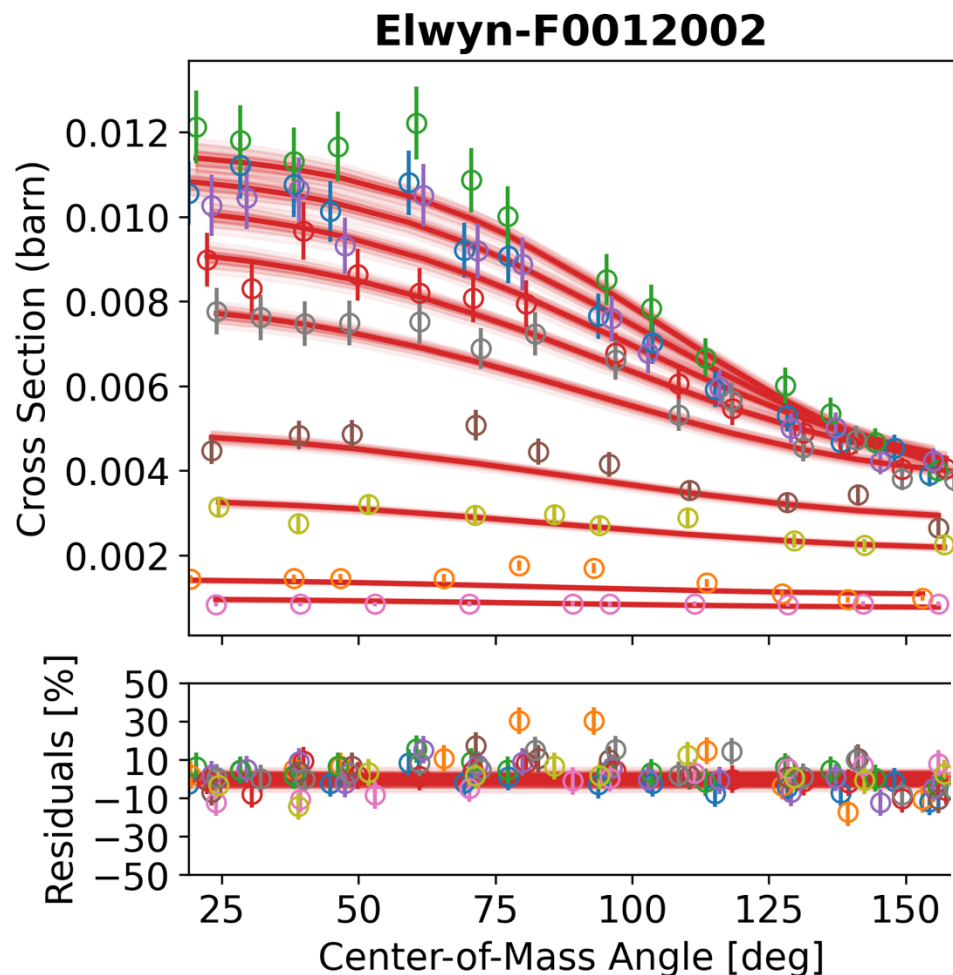
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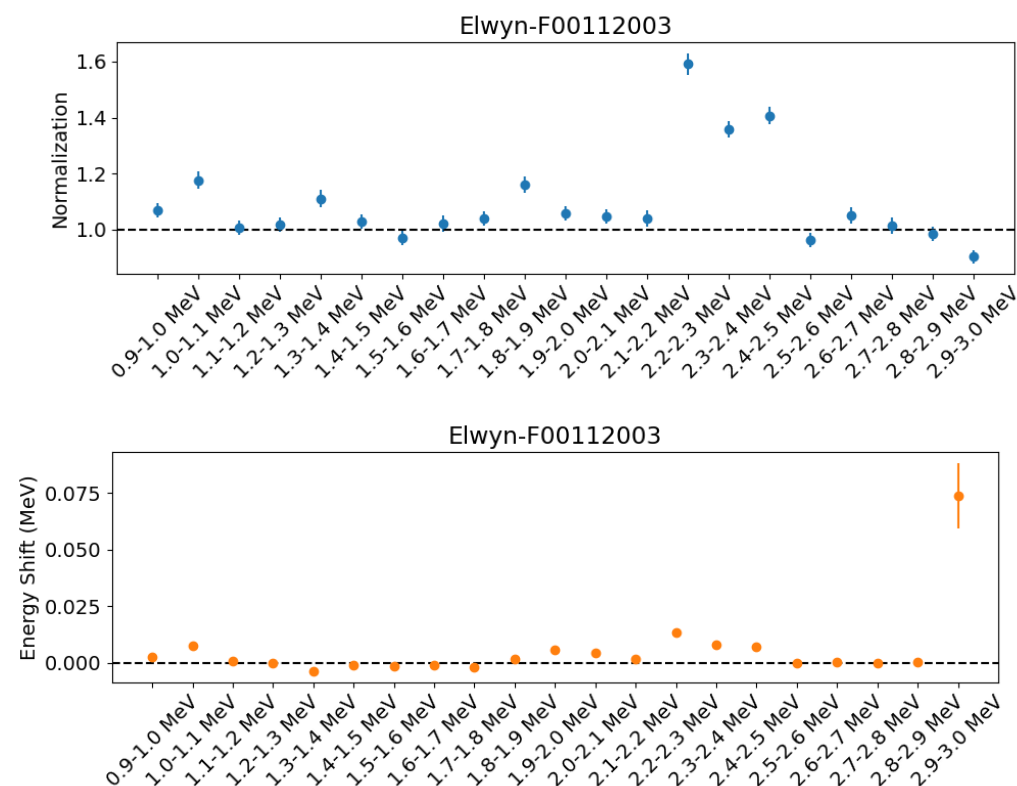
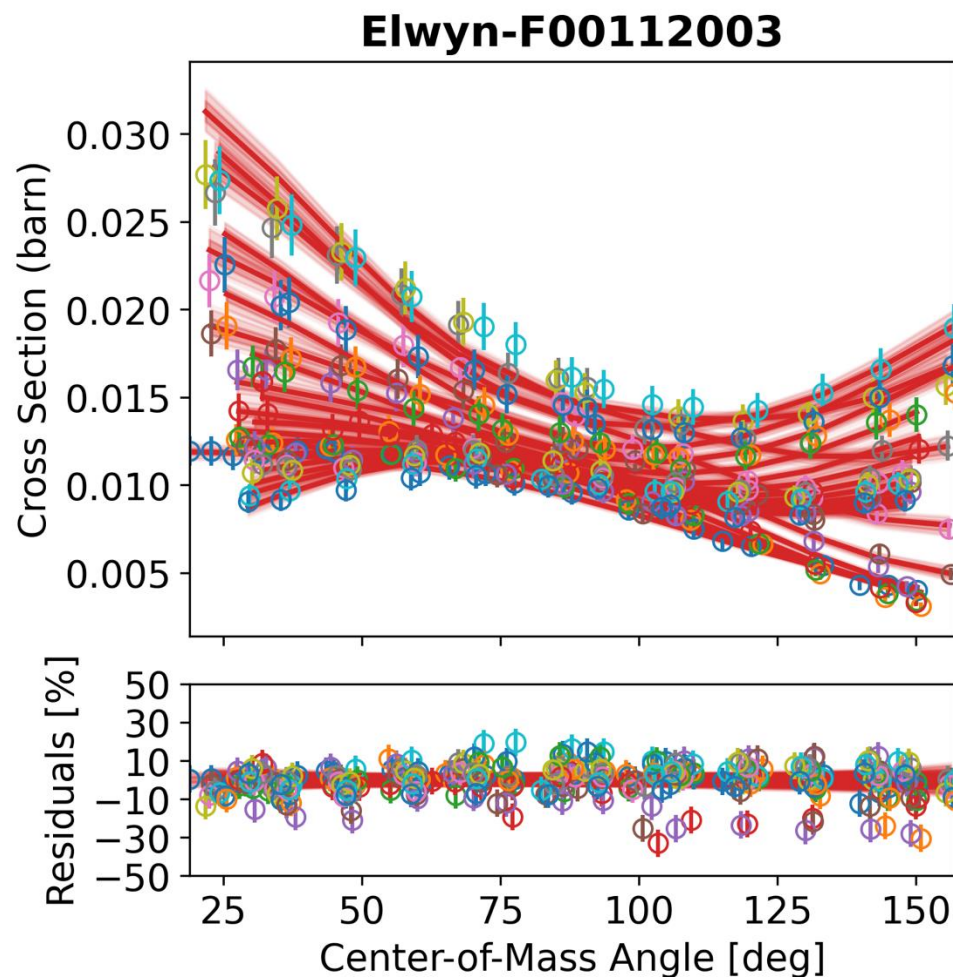
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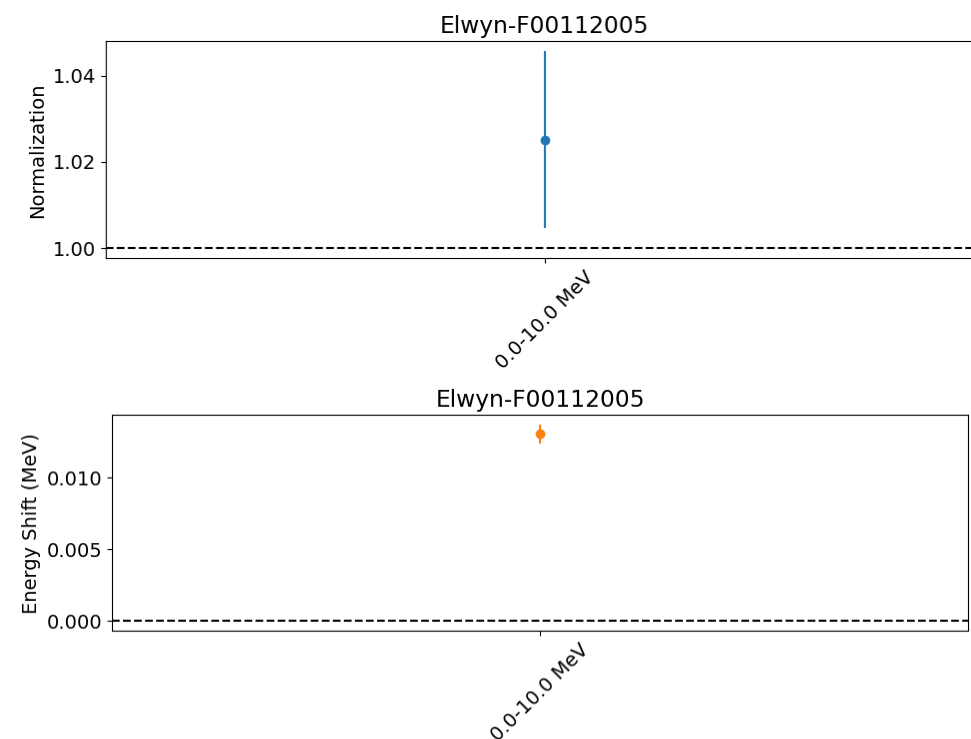
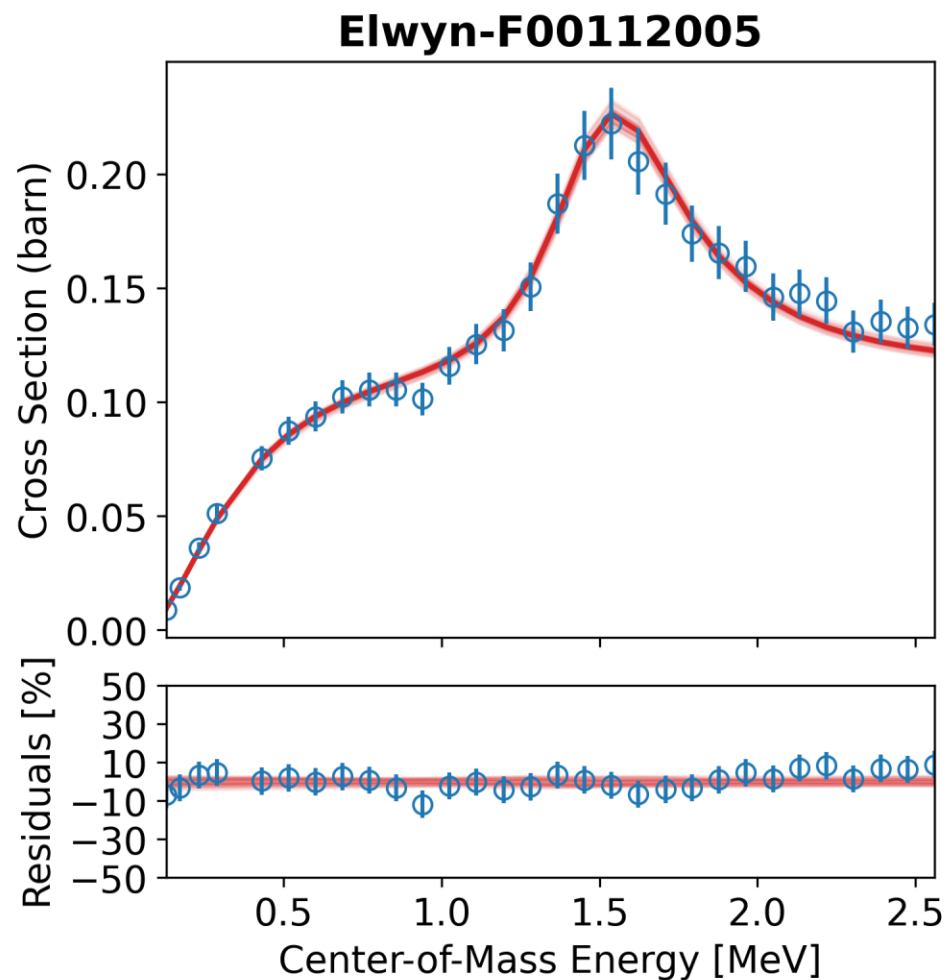
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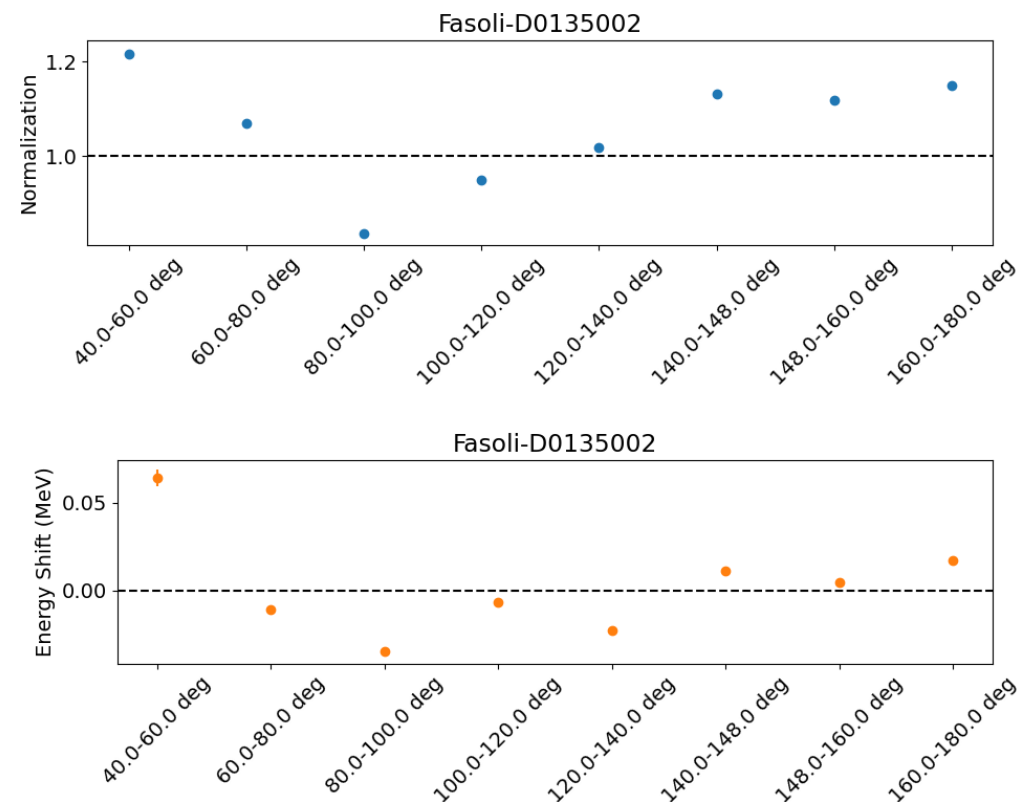
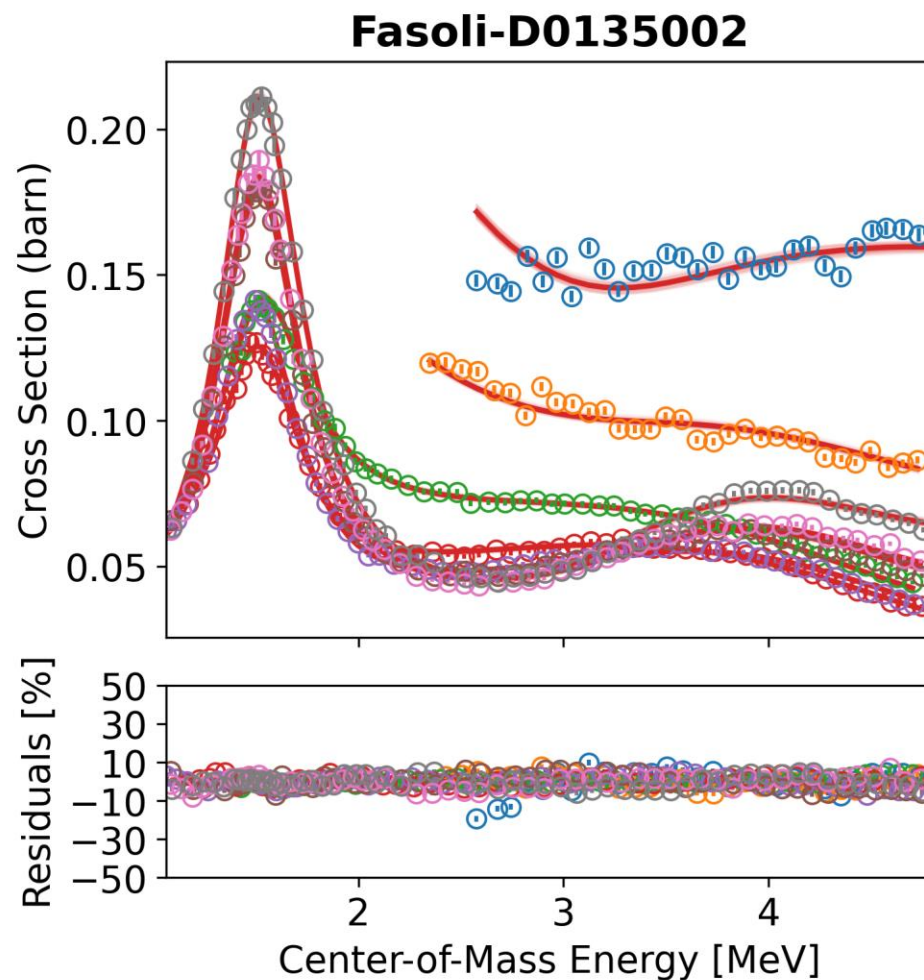
Tumino (O1221002)



^7Be Evaluation with AZURE2: Segments

Datasets

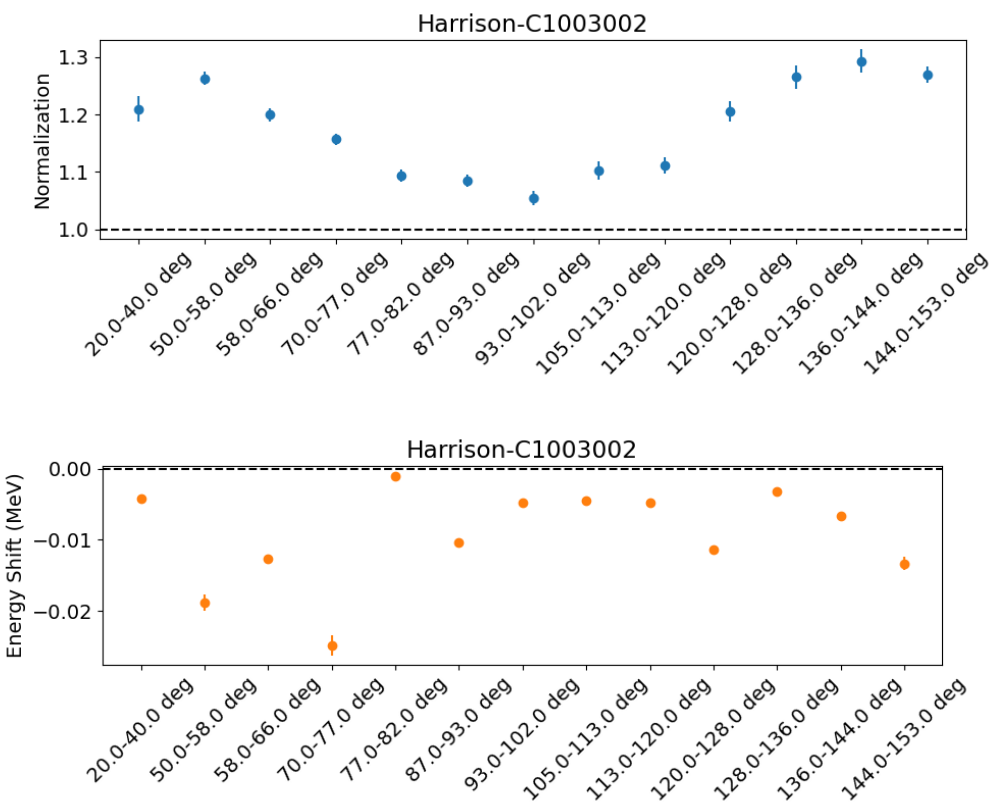
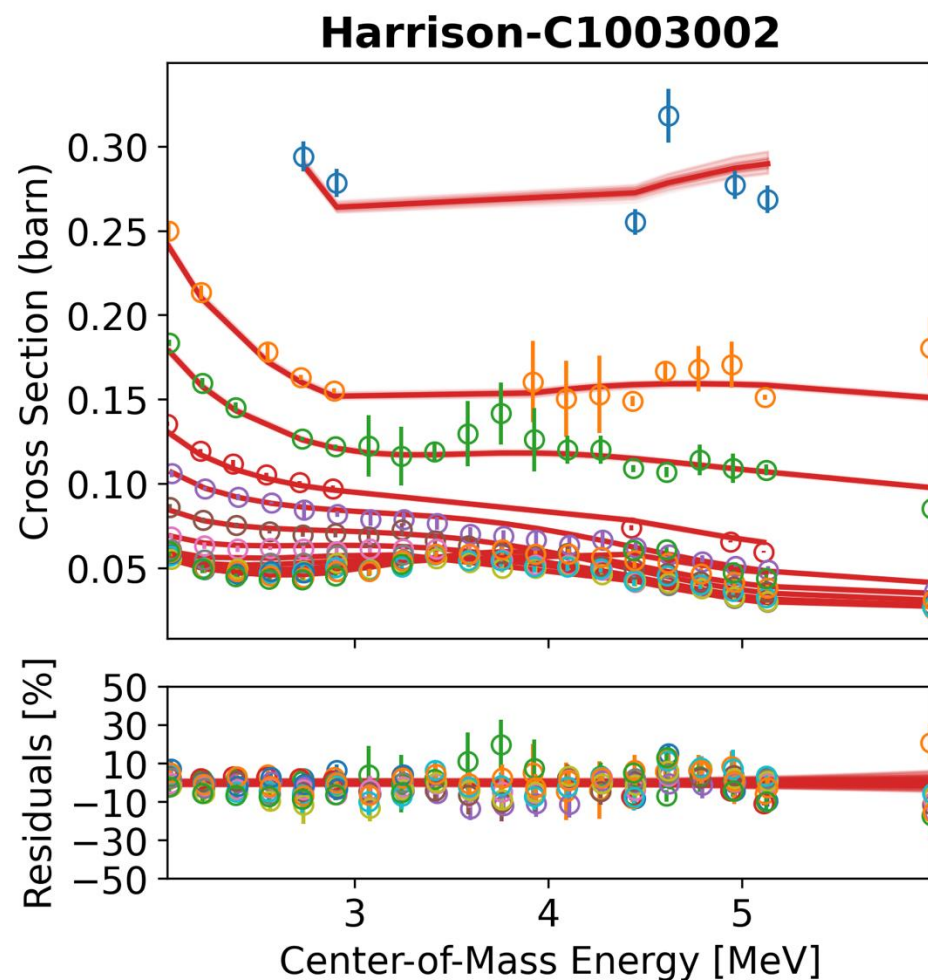
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^7Be Evaluation with AZURE2: Segments

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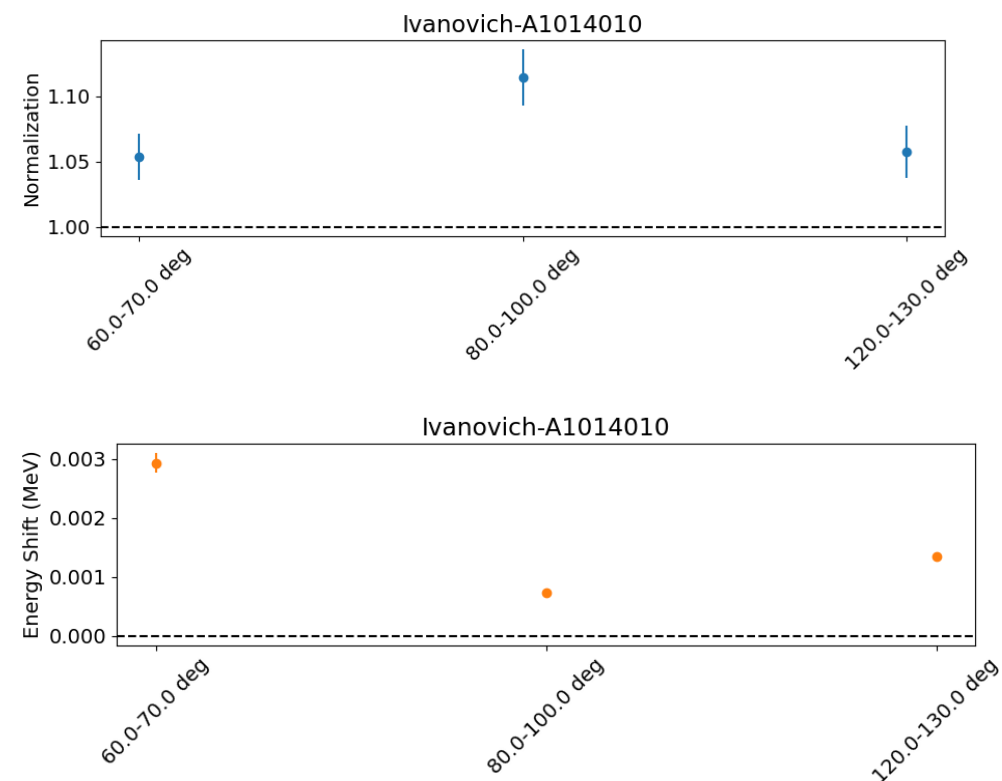
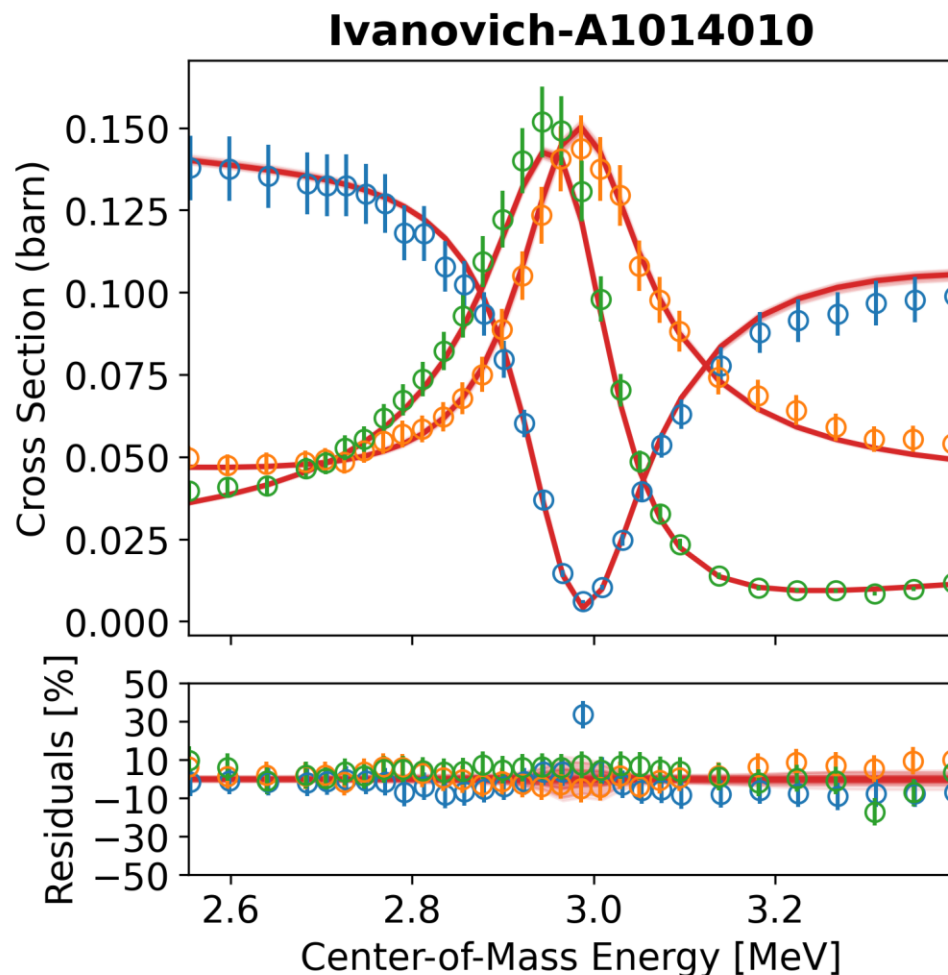
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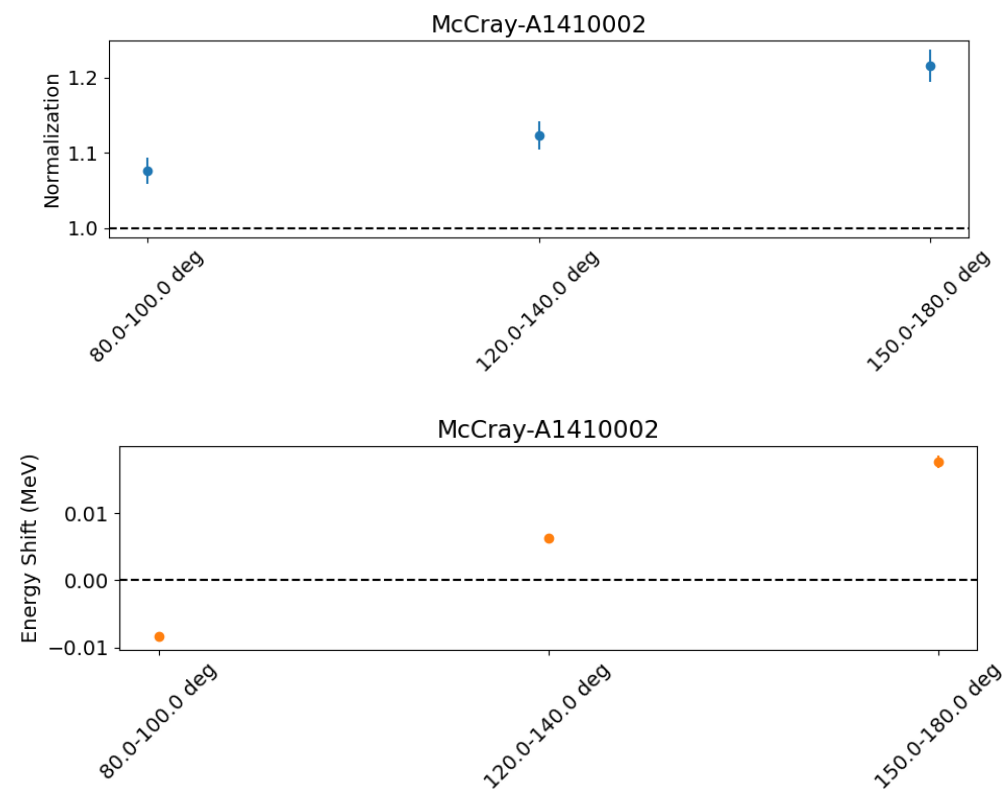
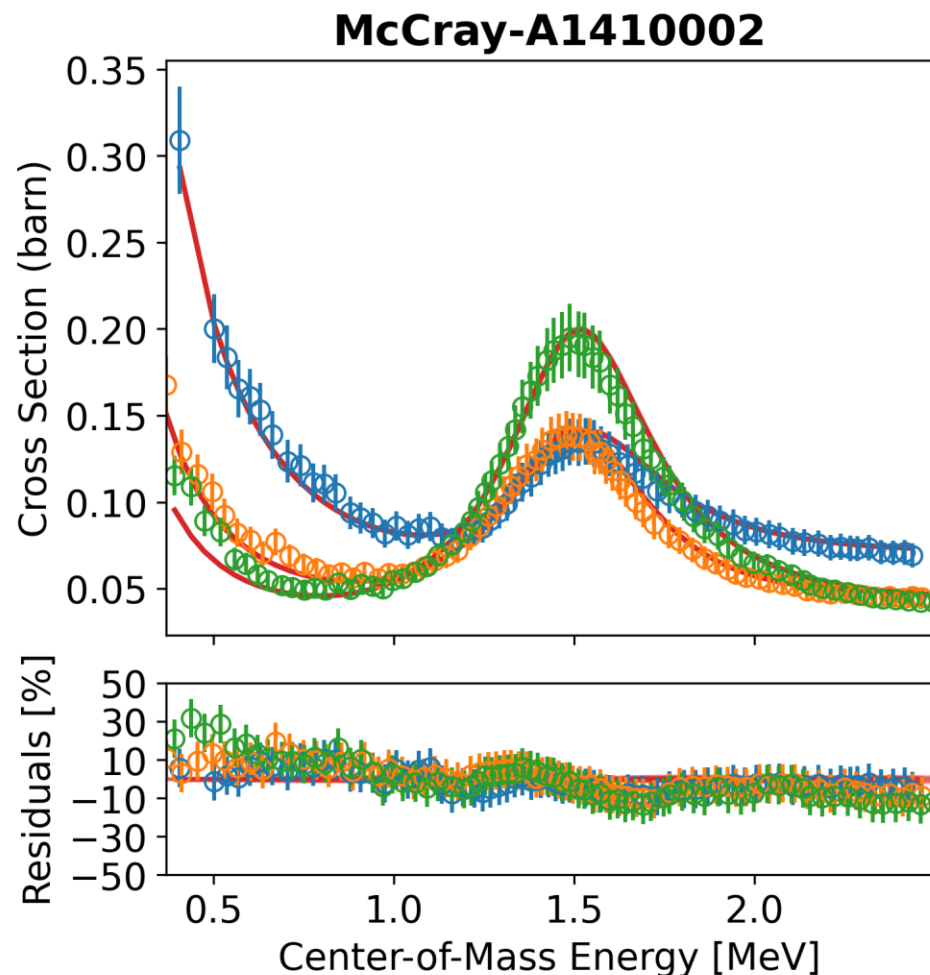
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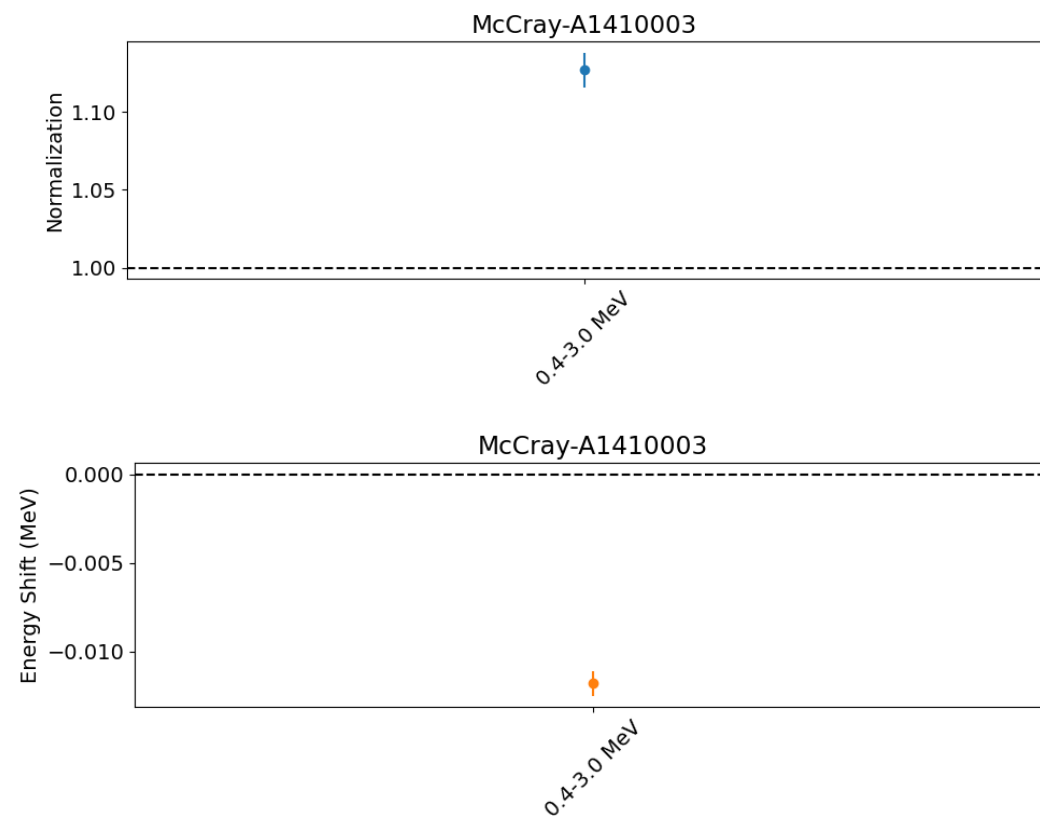
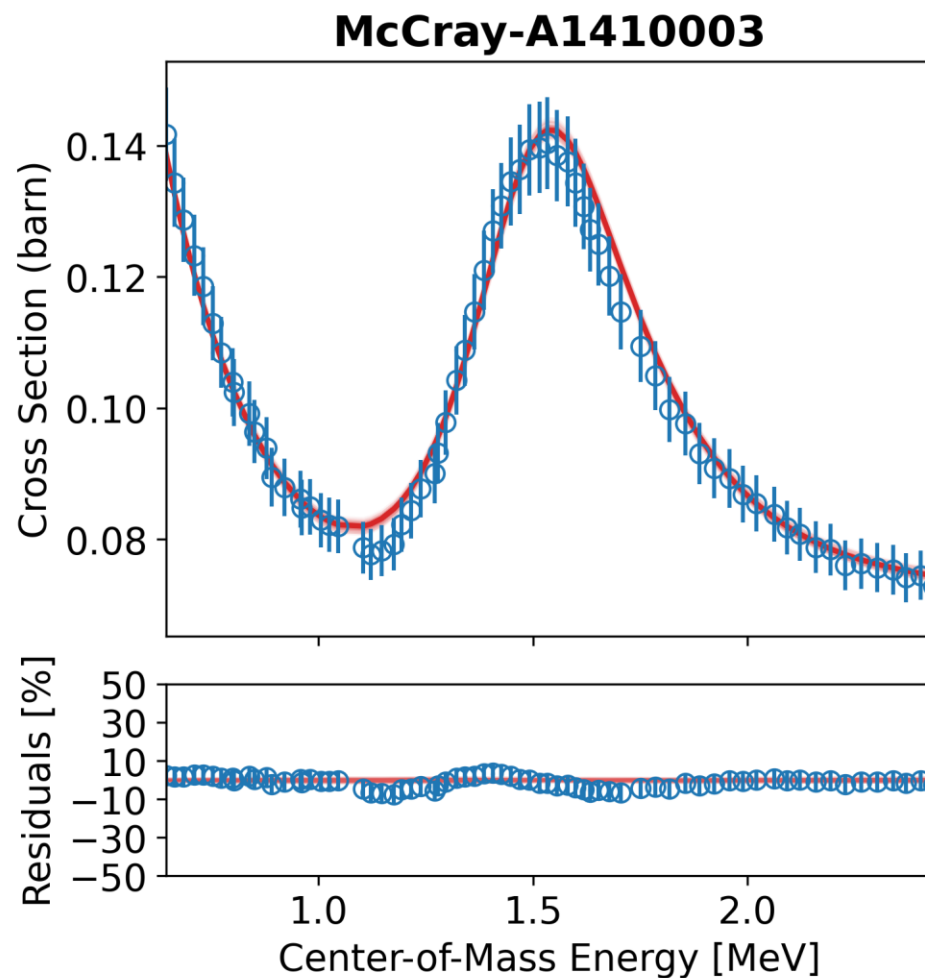
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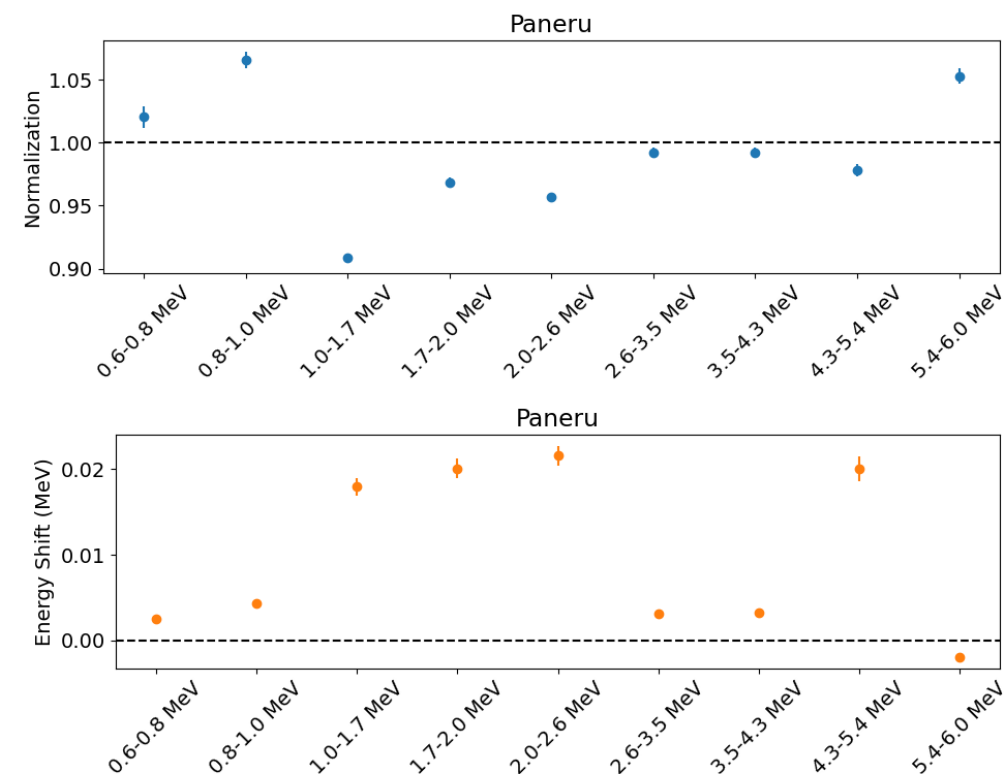
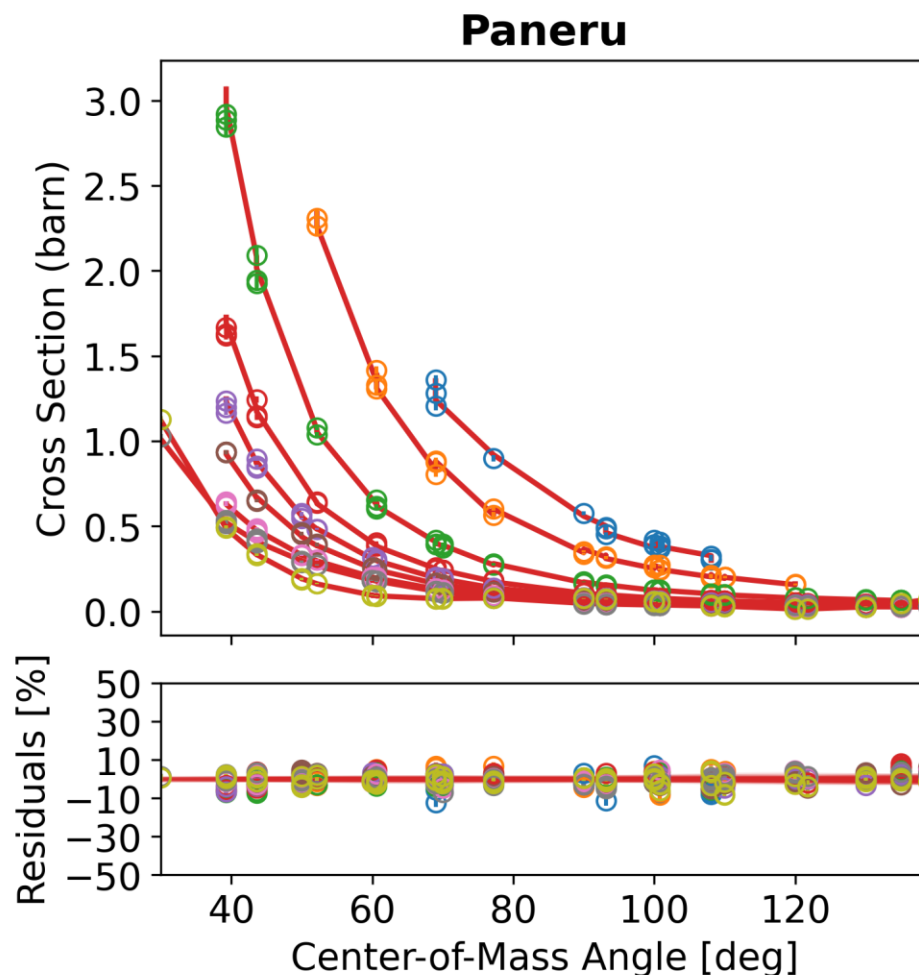
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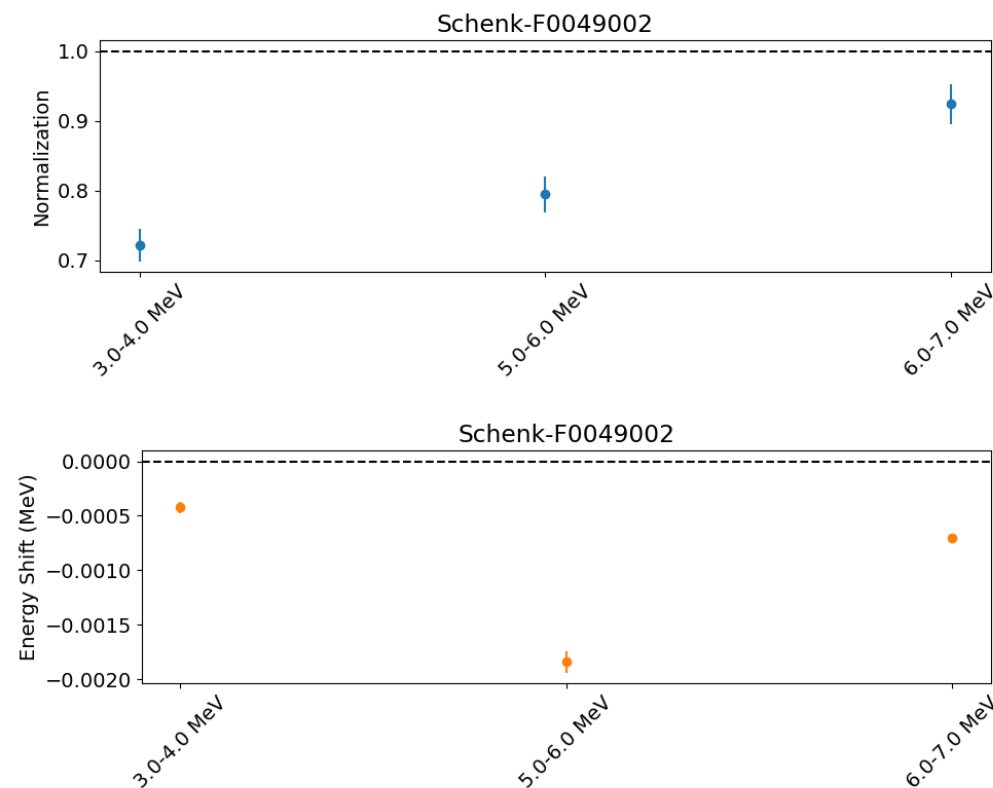
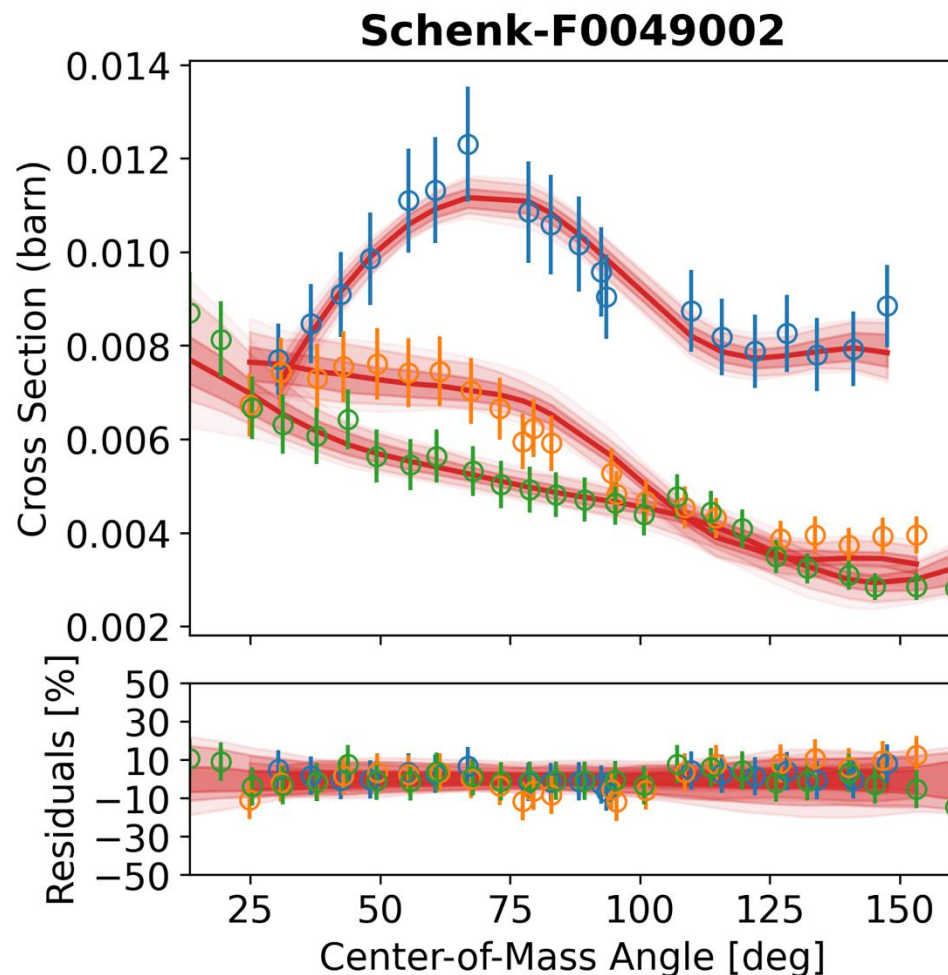
McCray (A1410002/3)

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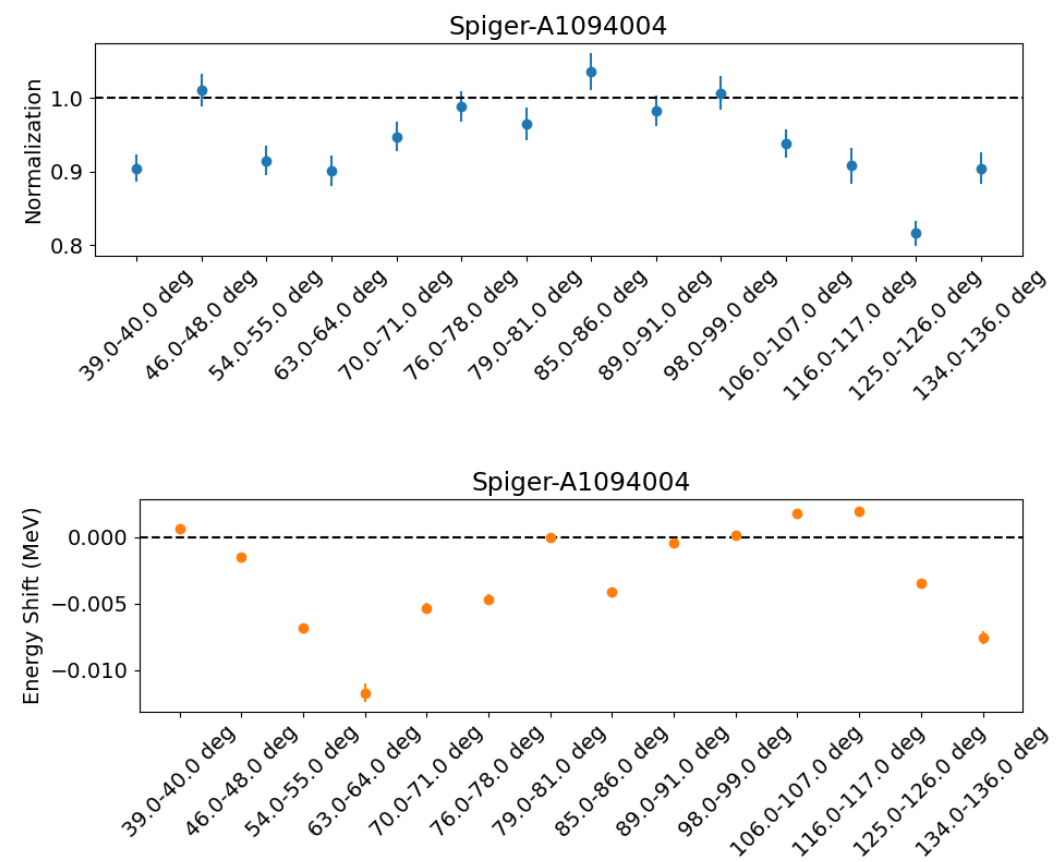
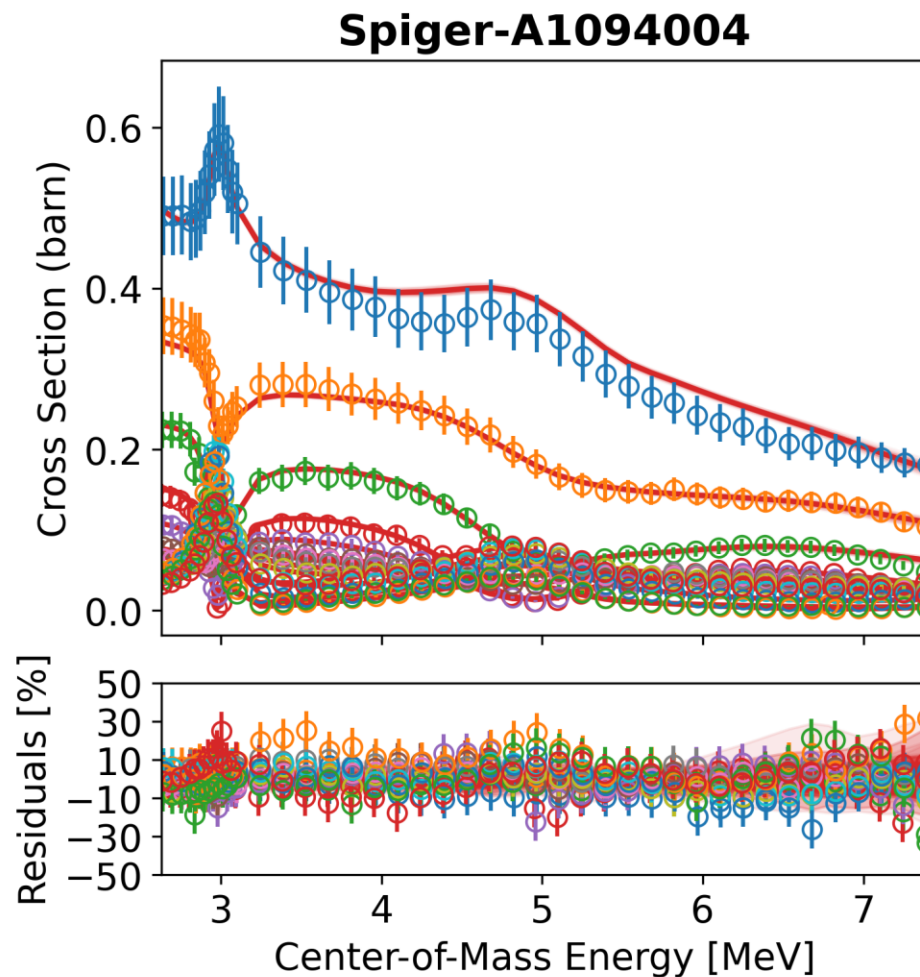
Tumino (O1221002)



^7Be Evaluation with AZURE2: Segments

Datasets

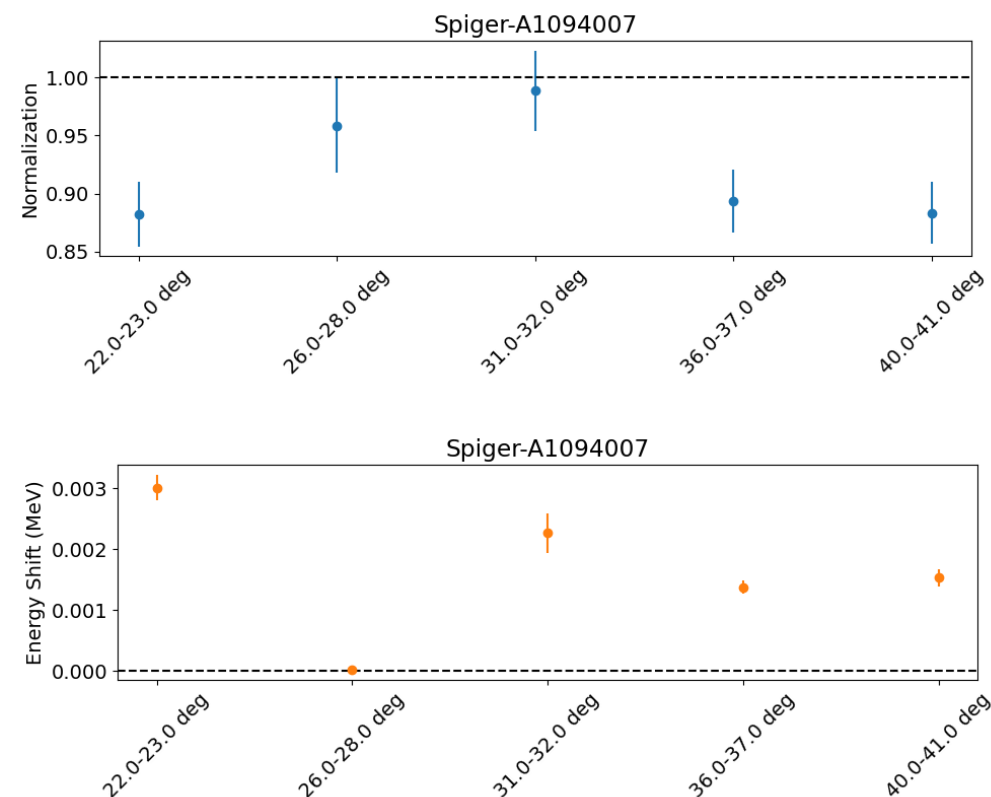
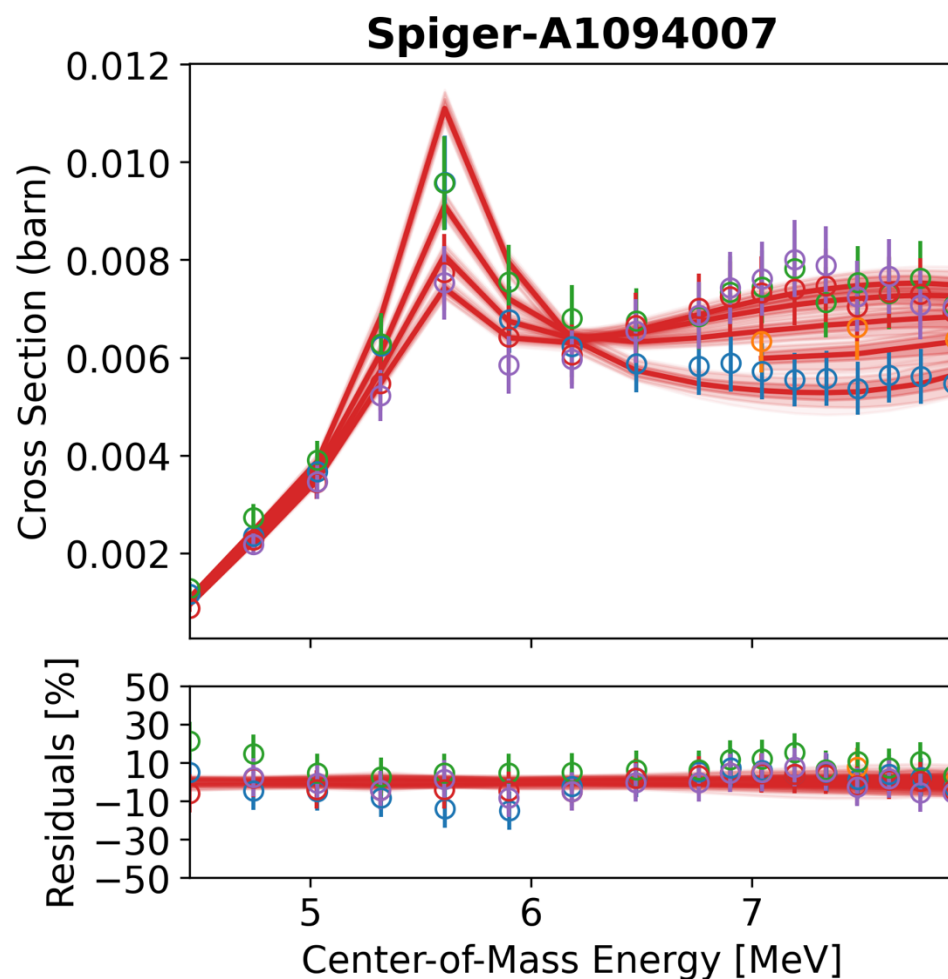
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^7Be Evaluation with AZURE2: Segments

Datasets

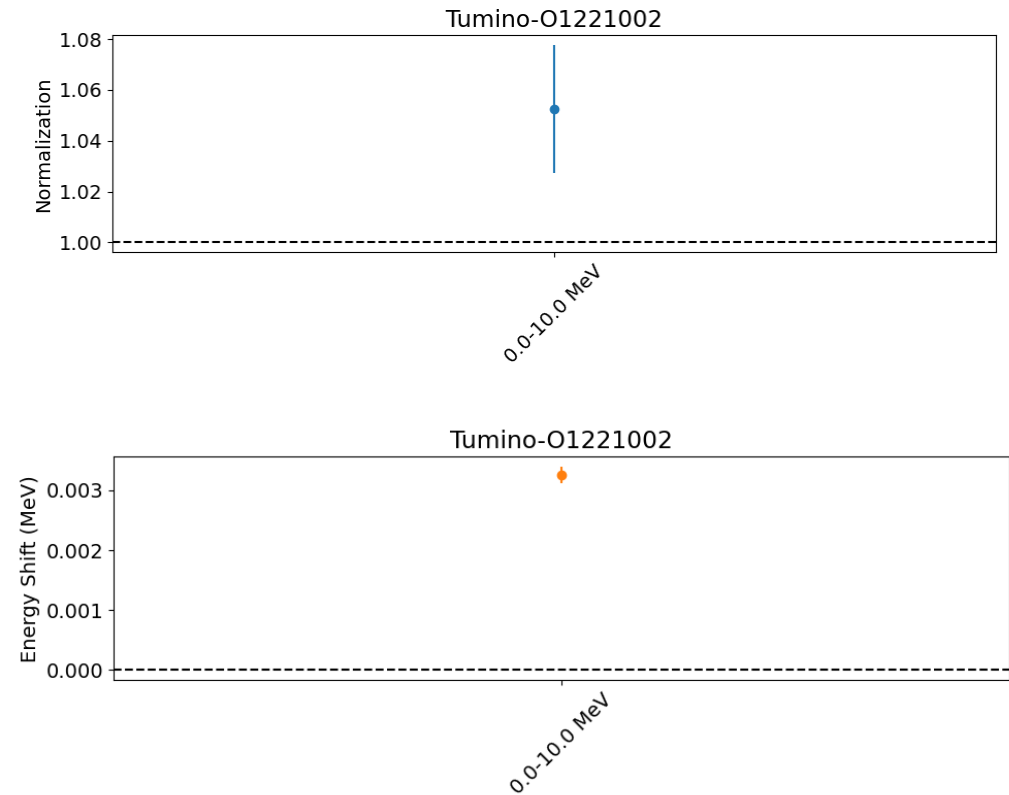
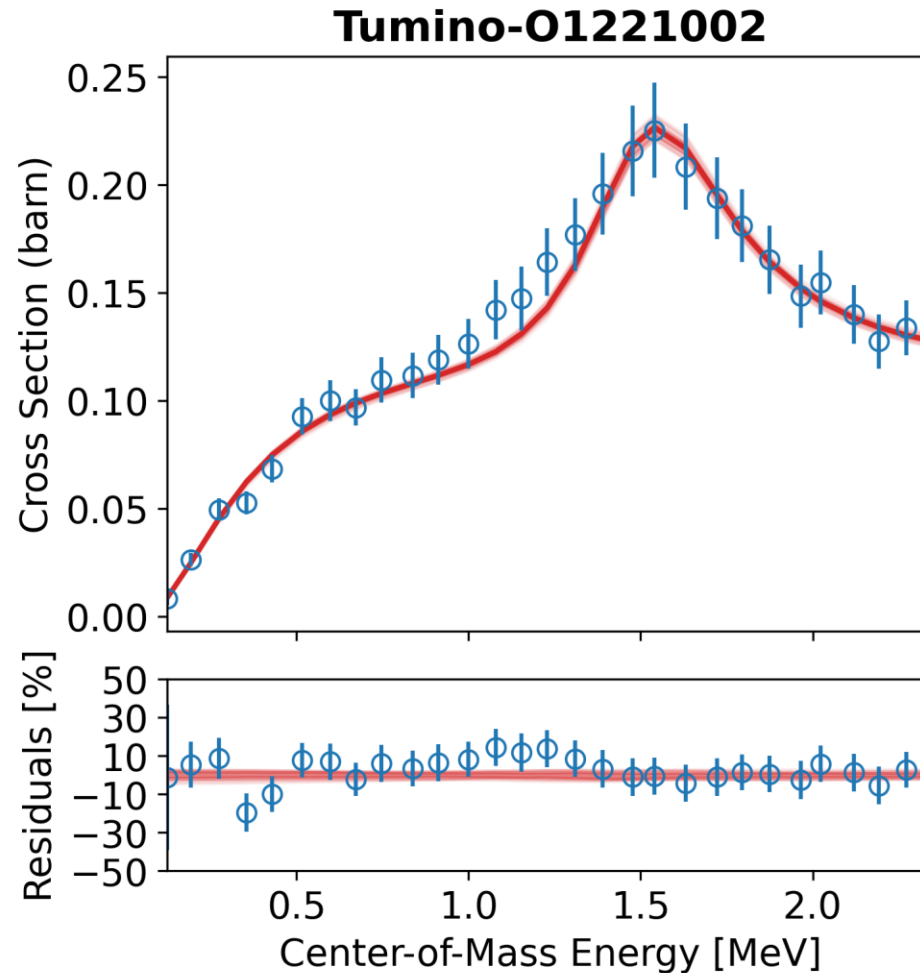
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^7Be Evaluation with AZURE2: Segments

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Conclusions

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

Conclusions

- In the last year AZURE2 got a lot of upgrades: **testing** and **paper in progress**
- The ^7Be evaluation is ready and reasonable: however, **background levels are needed**
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Thank you for attention!