A Data-driven Approach to Credible Uncertainty Quantification

Jacob Forbes, Elan Park-Bernstein, Cole Frisch, Justin Loring, Aaron Clark, Vladimir Sobes

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*Some figures are based on work of former students: Noah Walton and Jordan Armstrong

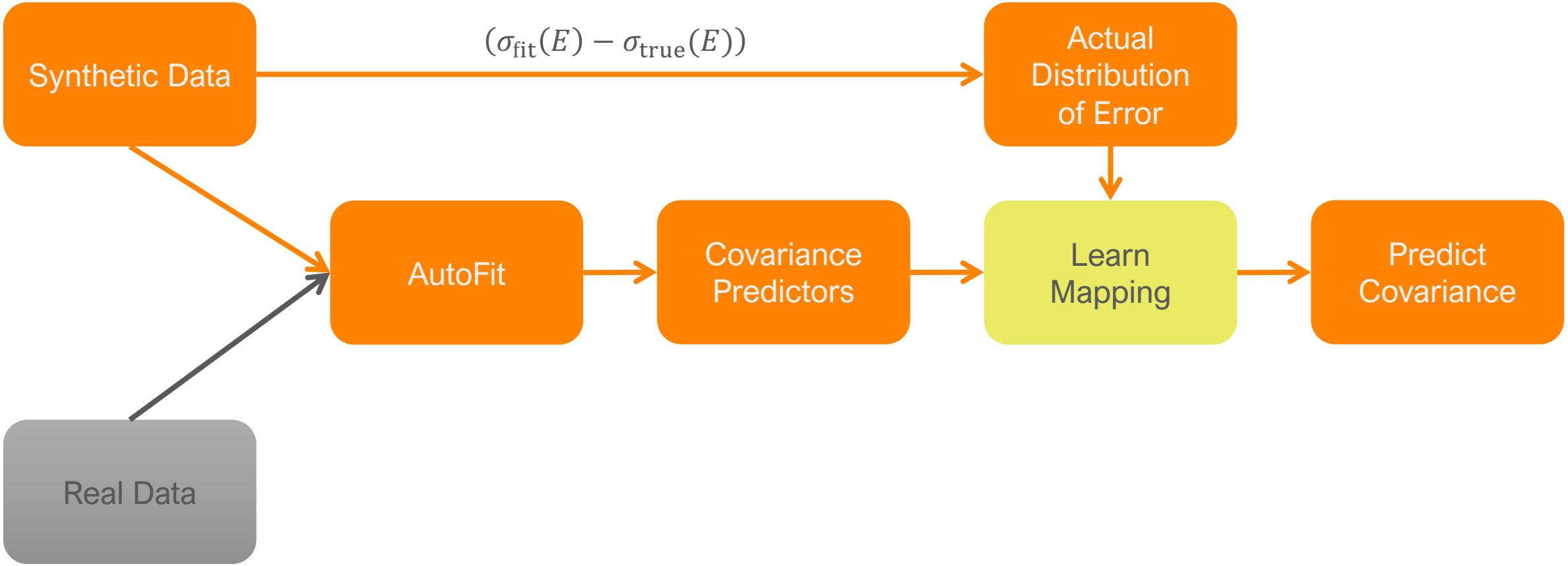
Main findings

Cross section uncertainty ~10% in RRR with good differential data

Access to distribution of error

Quantifiable impact on benchmarks / applications

Approach Overview



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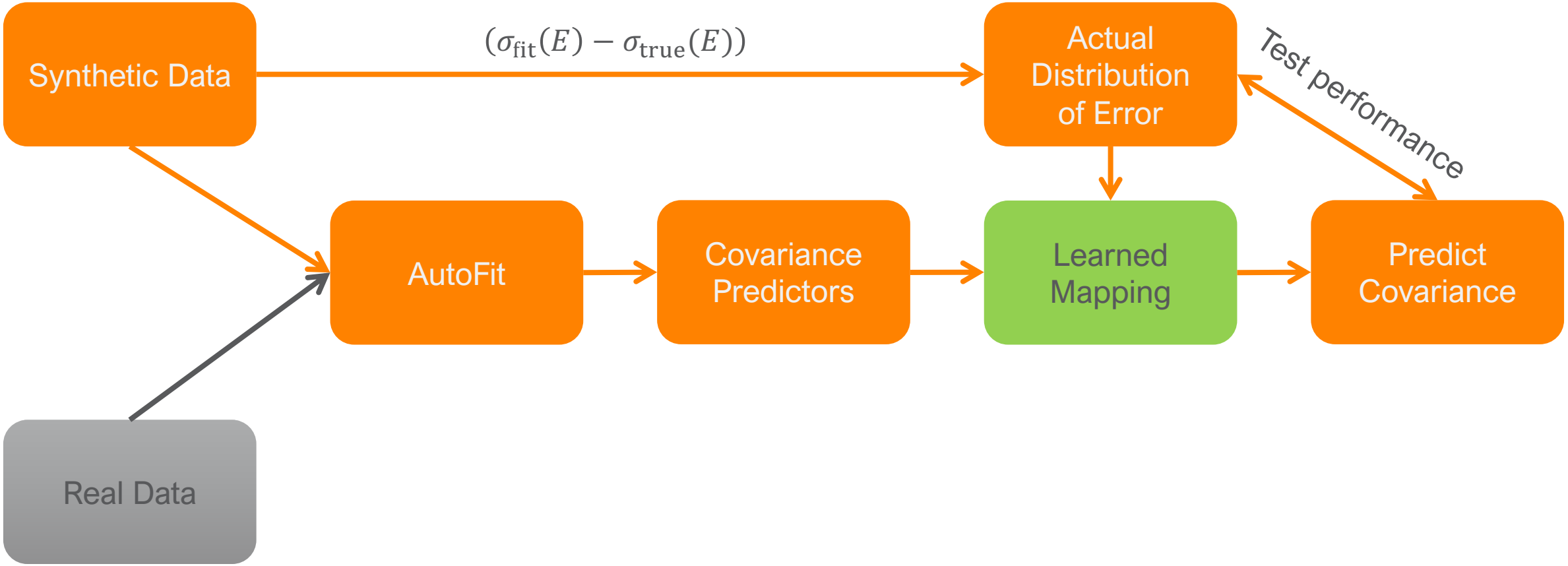

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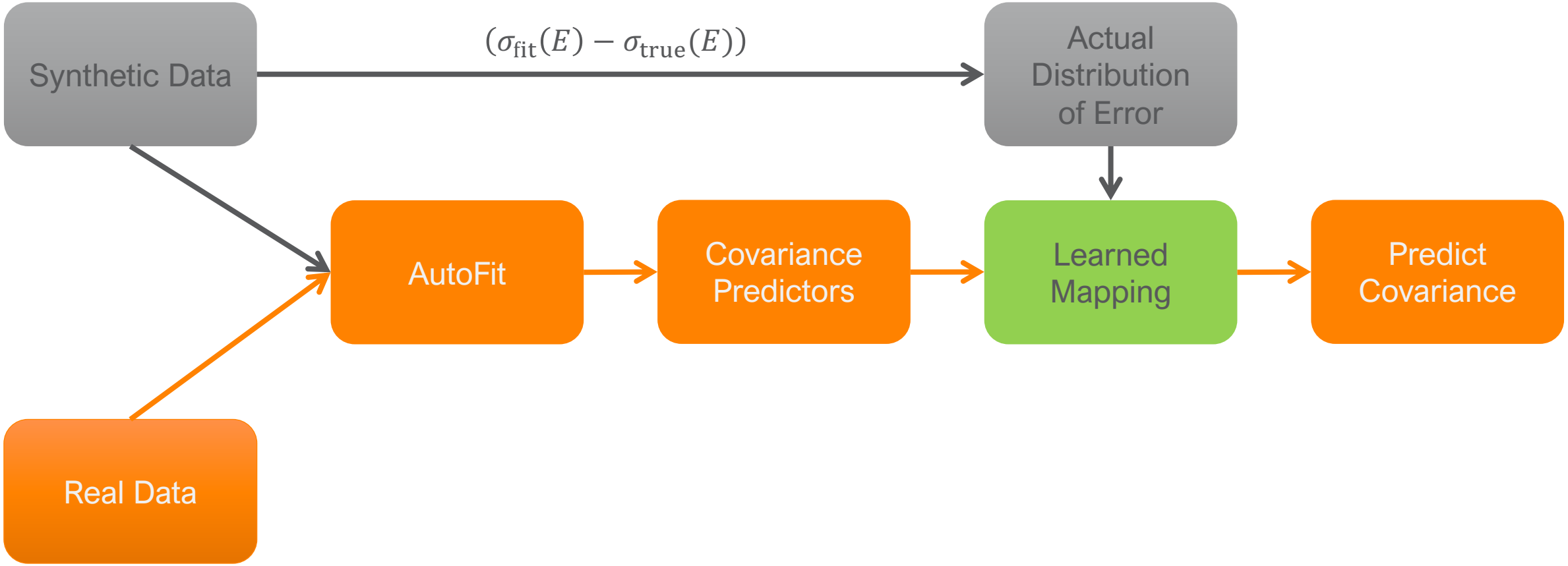
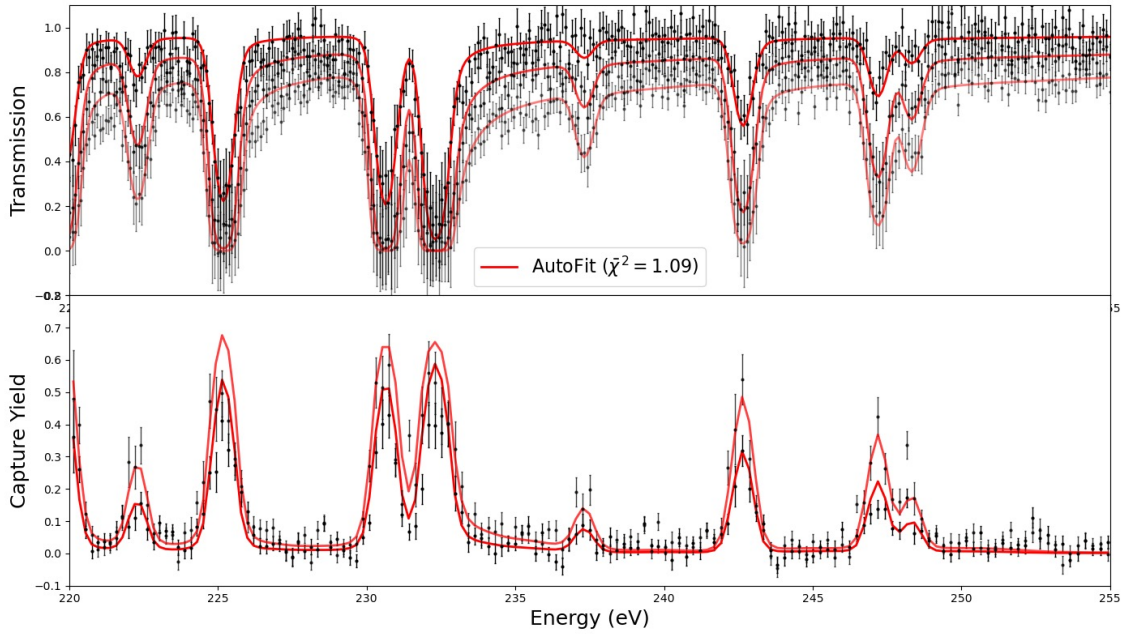


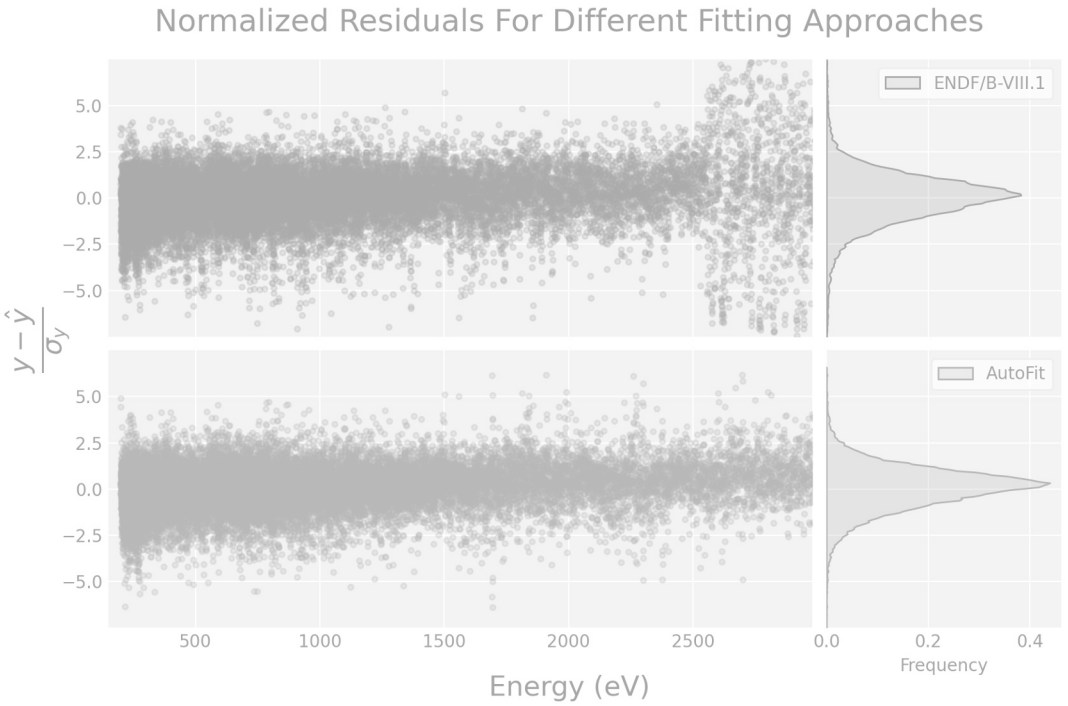
AutoFit Algorithm

Fitting Method	χ^2/N_{data}
AutoFit	1.354
ENDF/B-VIII.1	1.698
ENDF/B-VIII.1 Fit	1.581

Automated, deterministic, repeatable

χ^2 fitting on par with human evaluators





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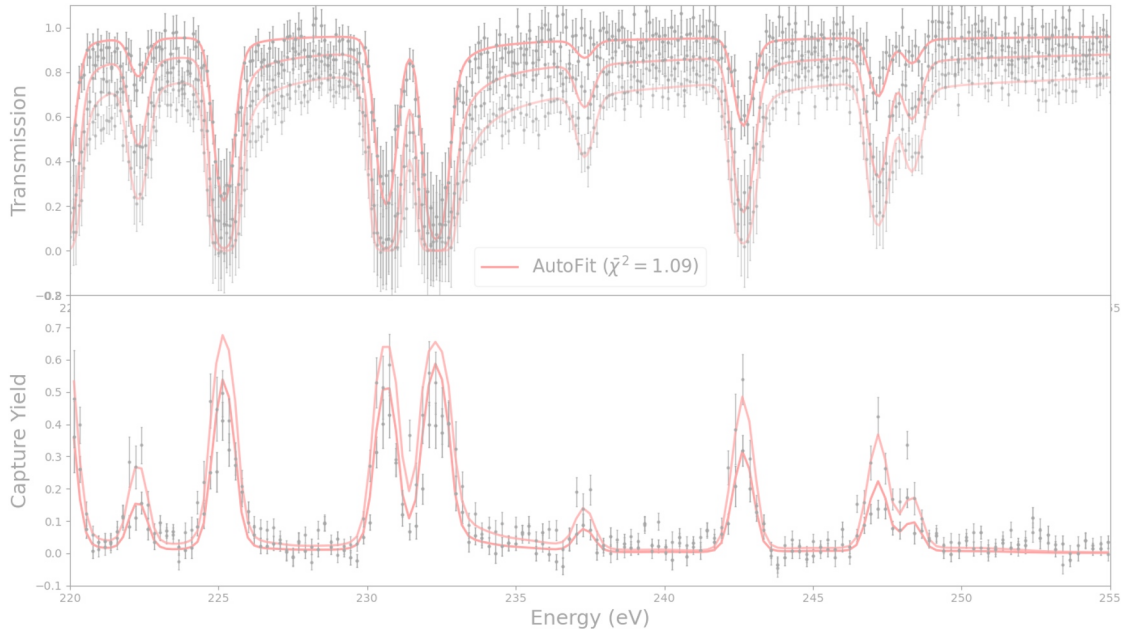
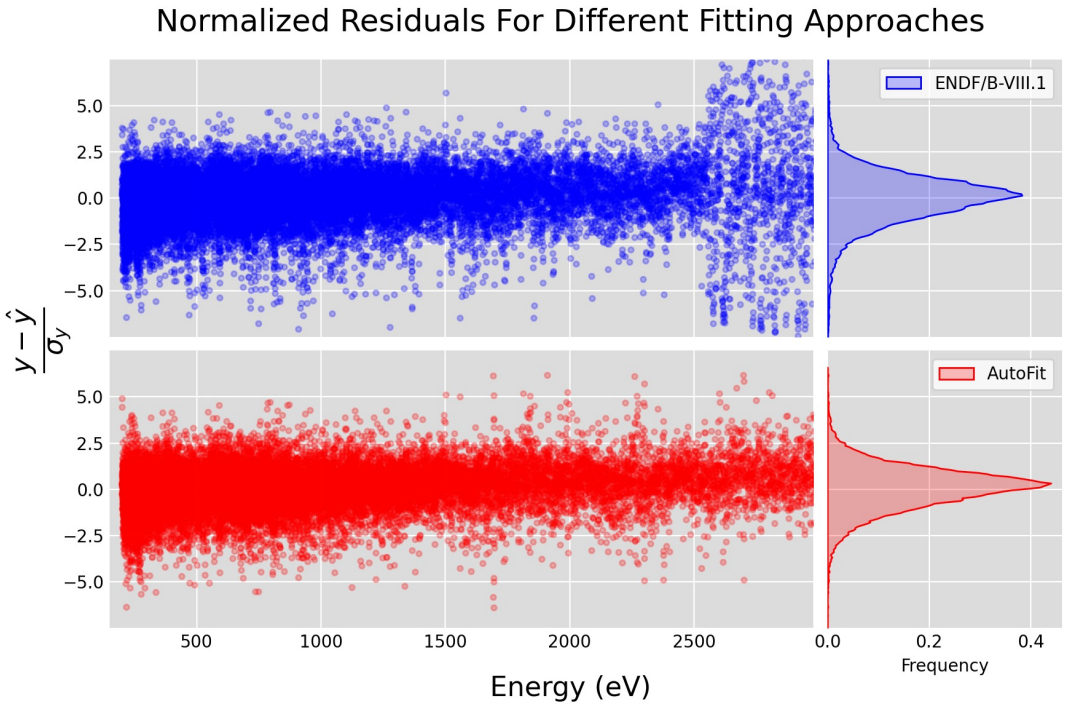
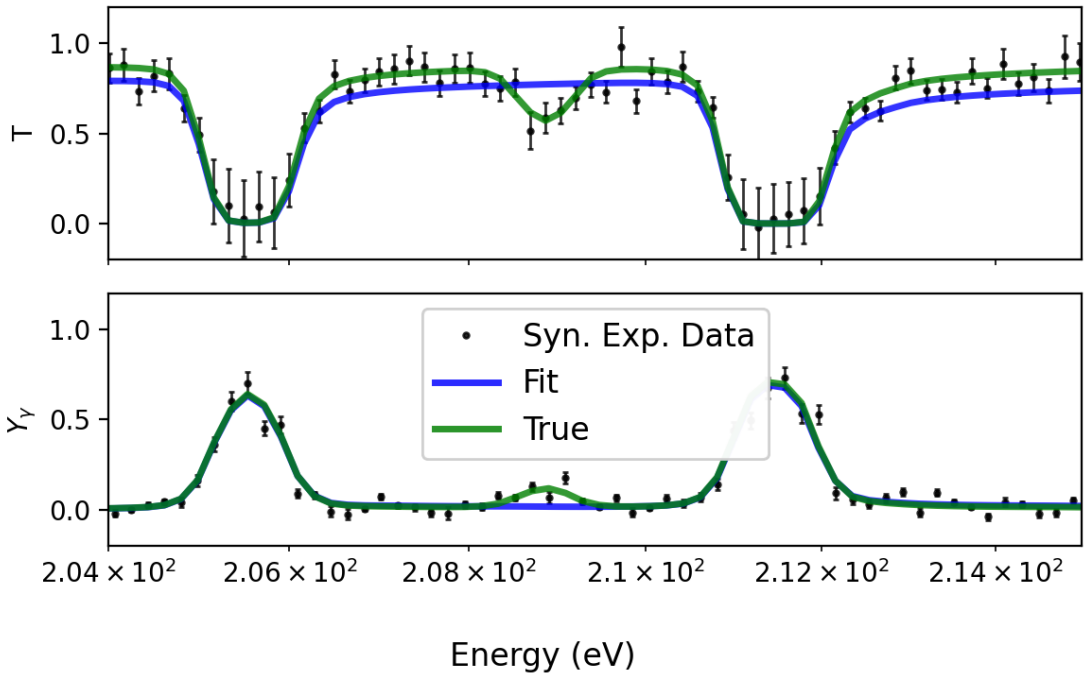
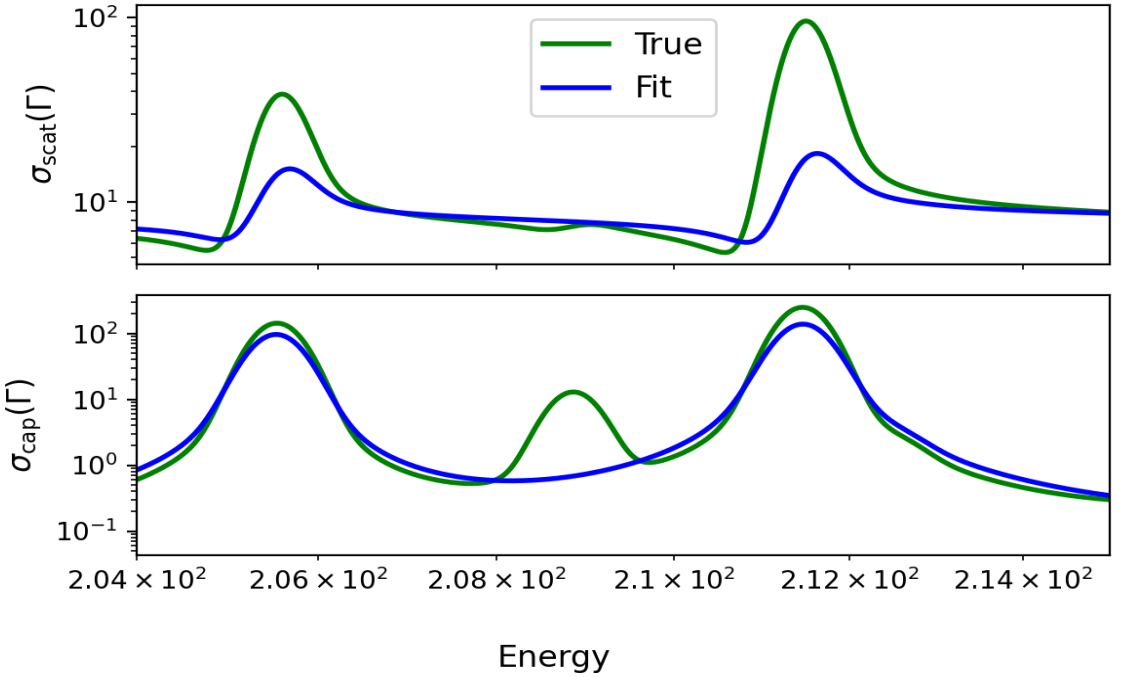




Why Synthetic Data?

- A repeatable test environment with **ground truth**
- “Best Case” scenario: all **Unknown Sources of Uncertainty can be controlled**
- Reveals the **true distribution of errors**





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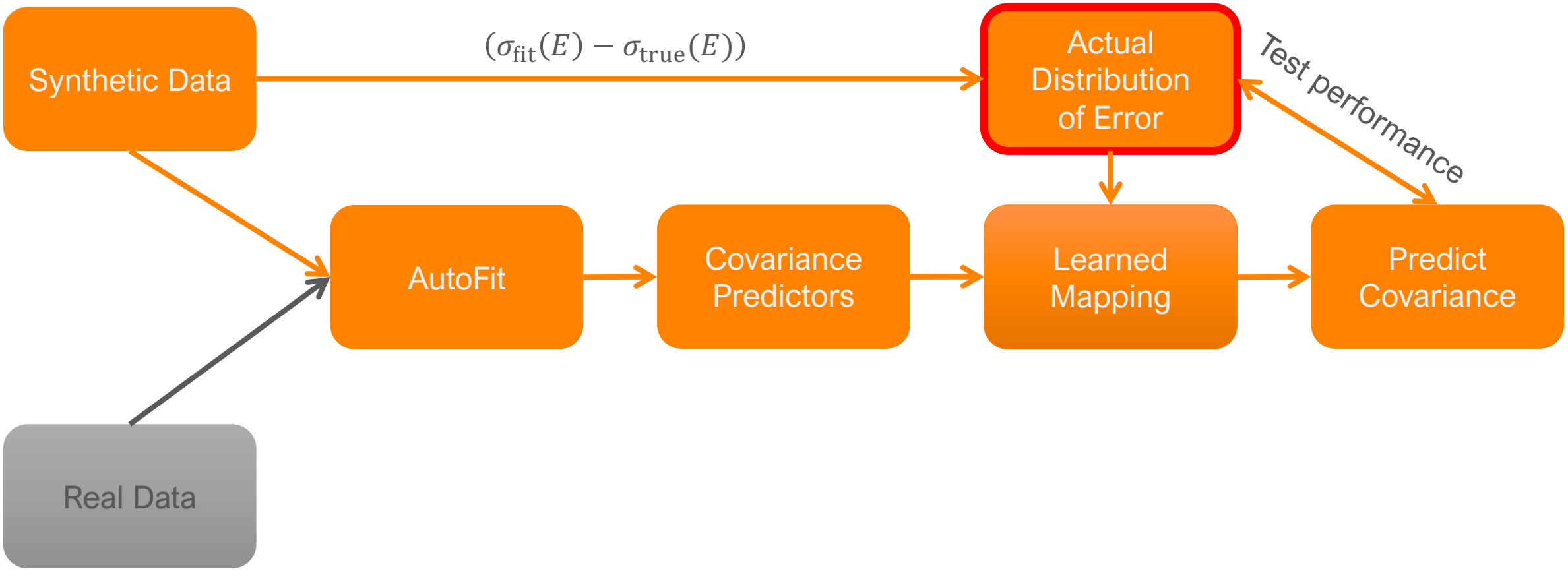


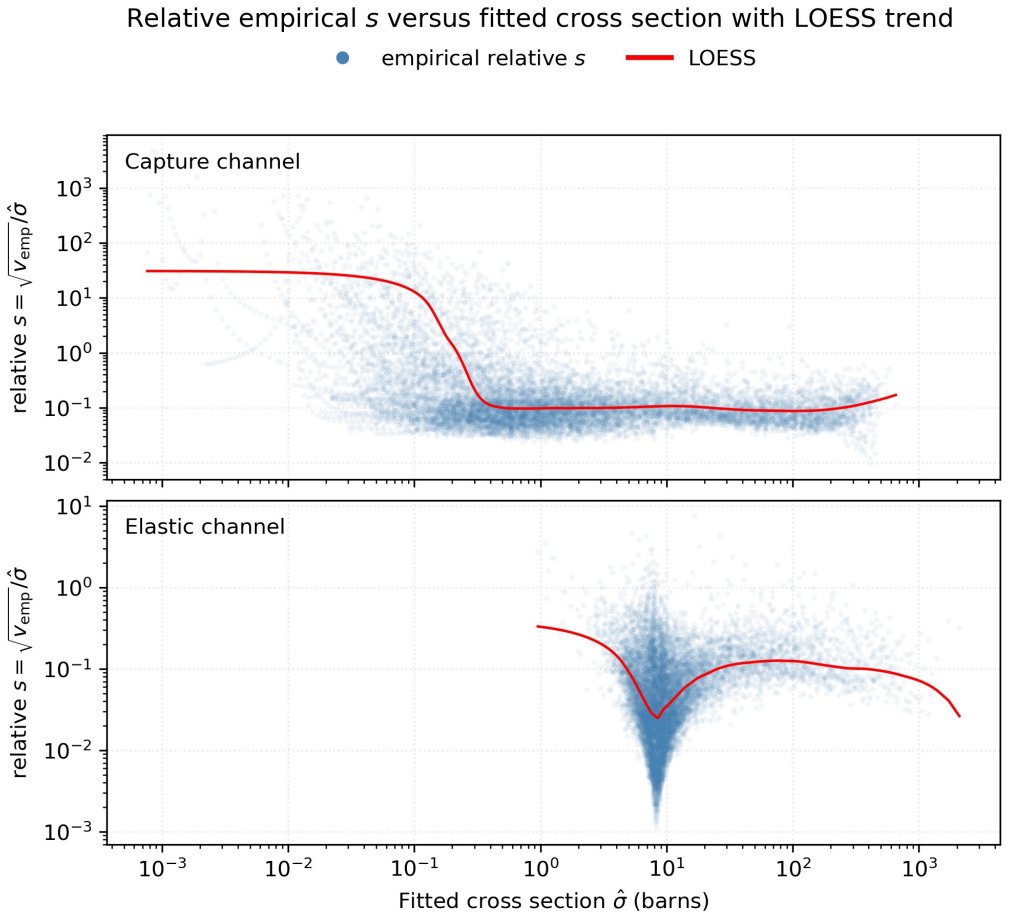
What Synthetic Data Tests Reveal

- 500,000 cross section fits
- 3 transmission data sets
- 2 capture yield data sets

~10% error in cross section

- Both capture and elastic
- Nearly independent of cross section value

  i.e.: resonance peak or valley



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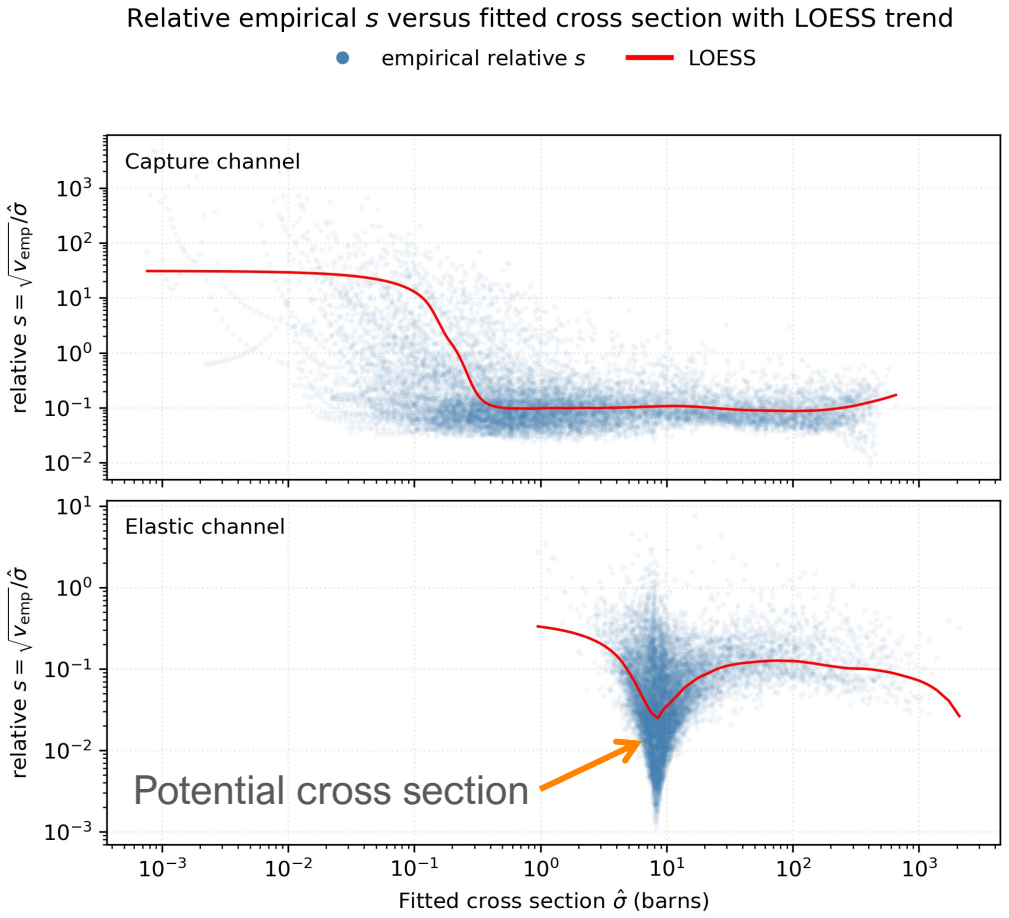
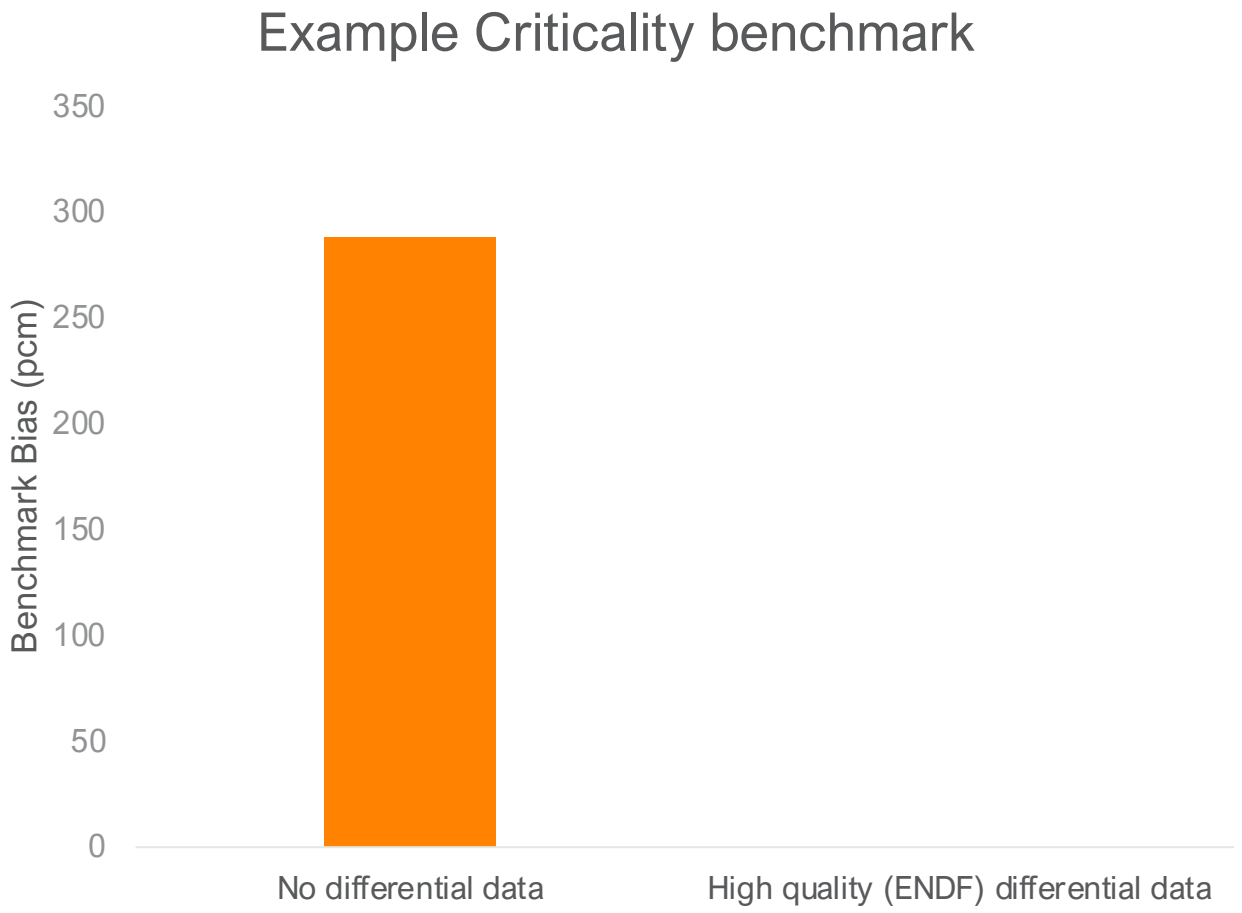
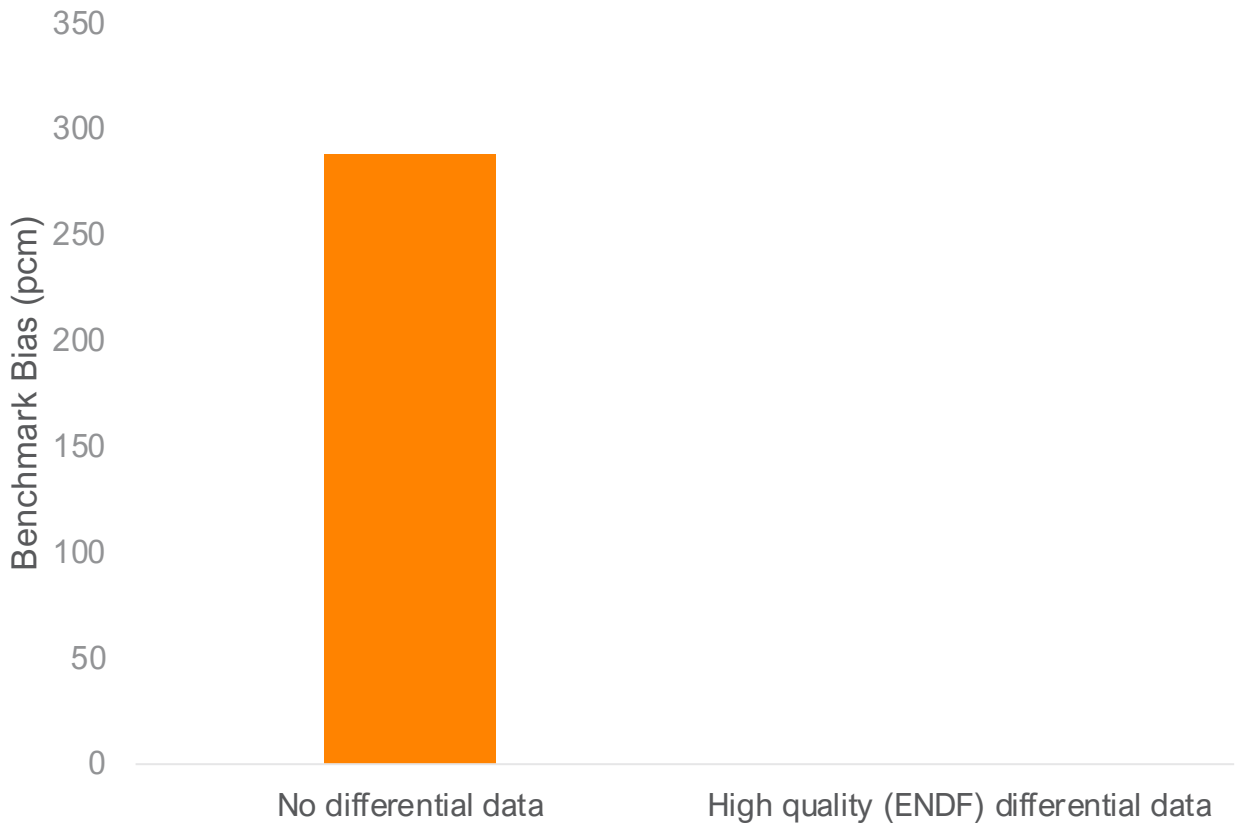


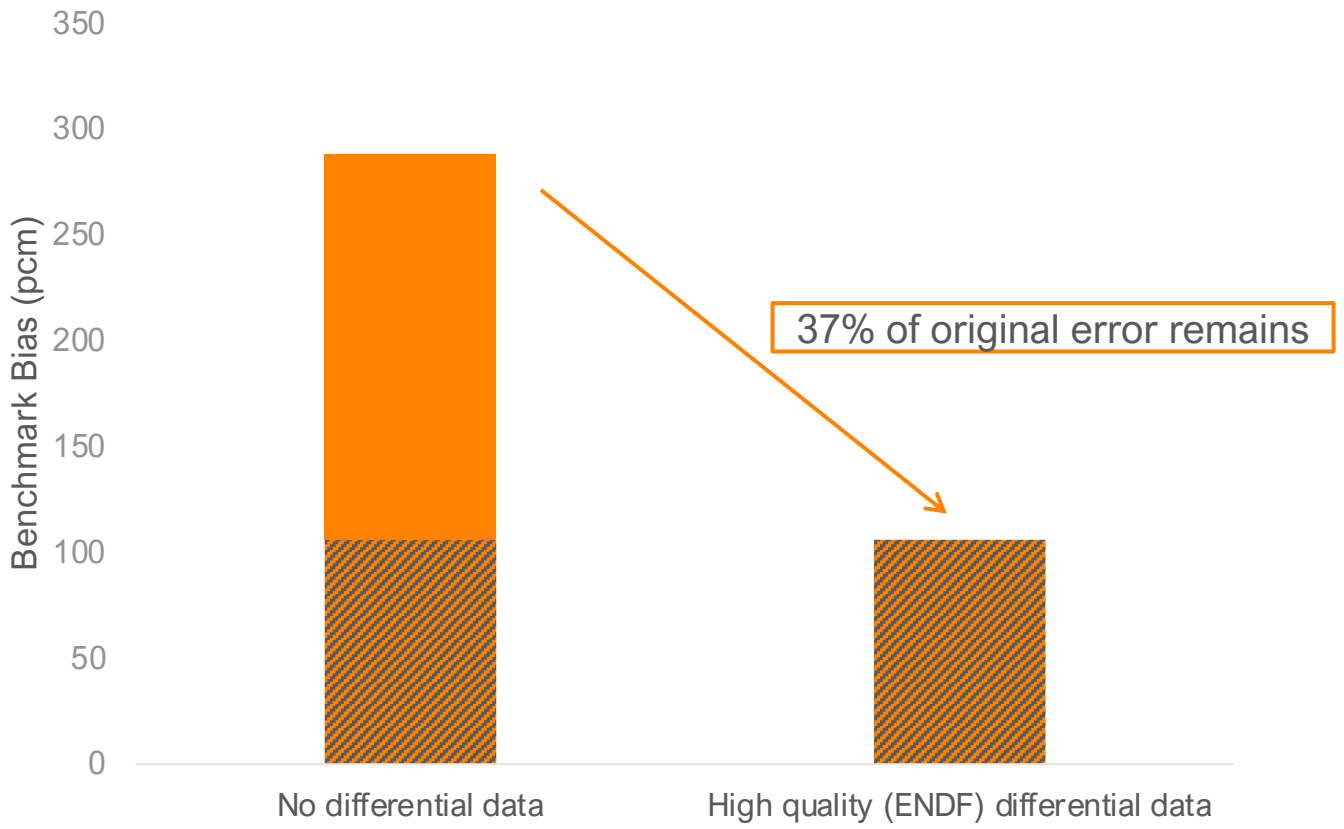


Example Criticality benchmark



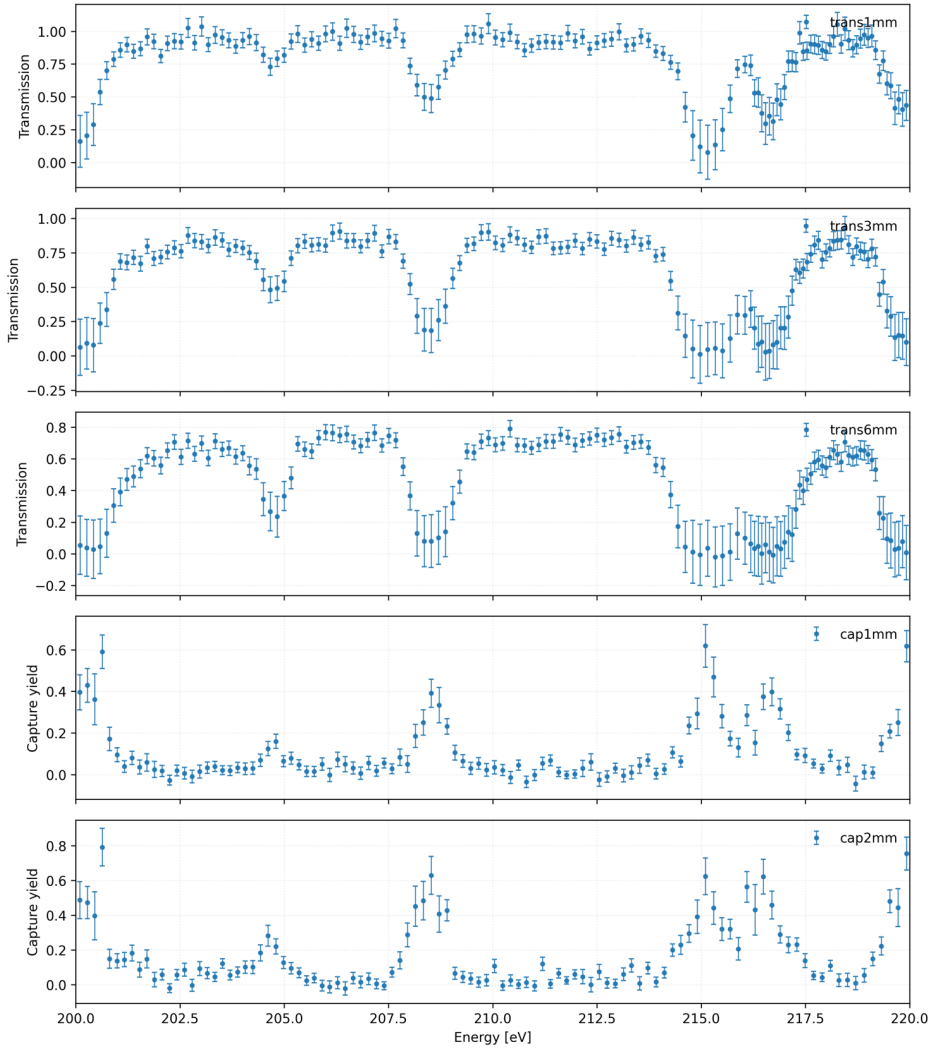
"URR-like" treatment
with known average parameter values

Example Criticality benchmark

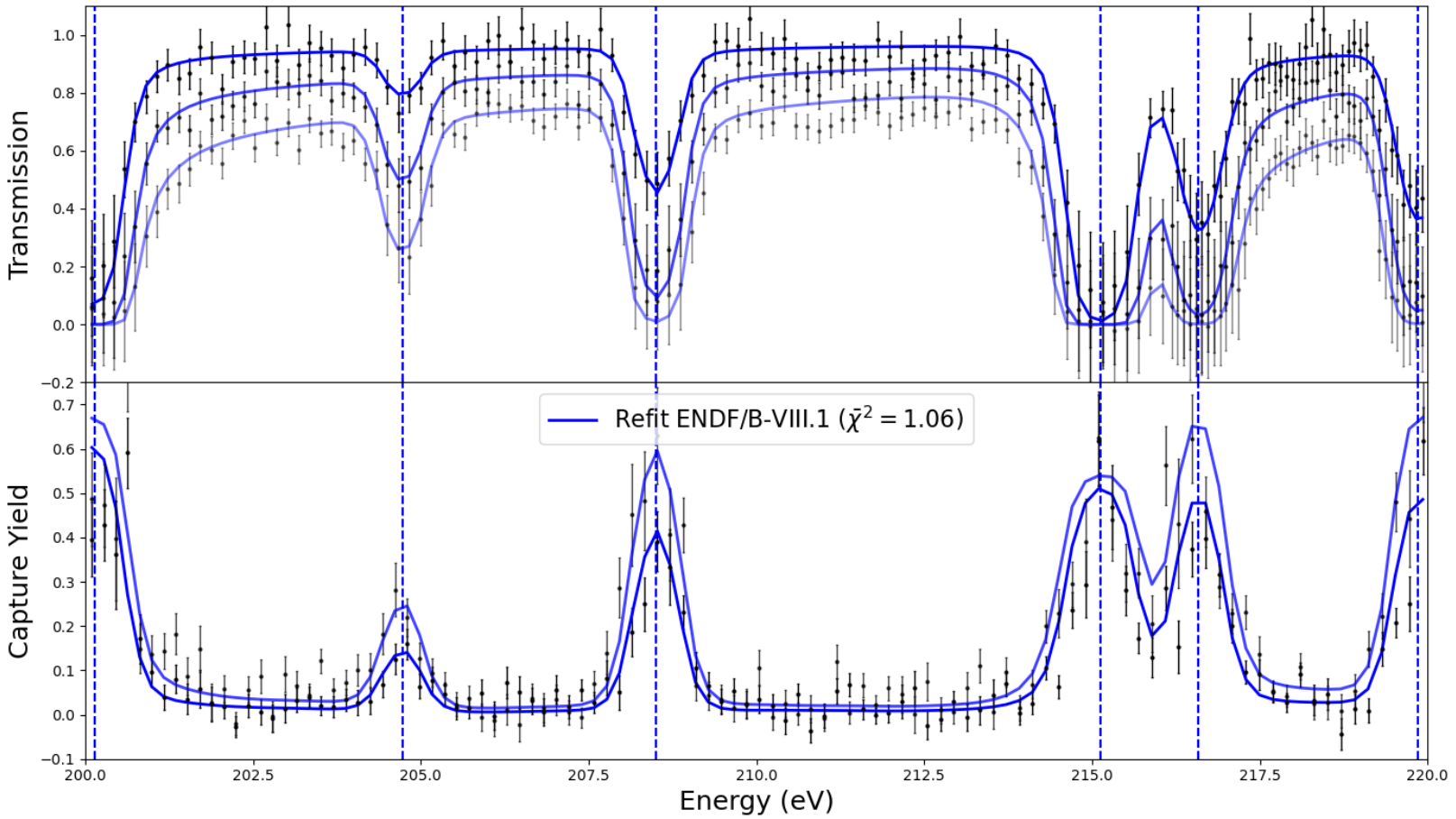


Transition to Real Data

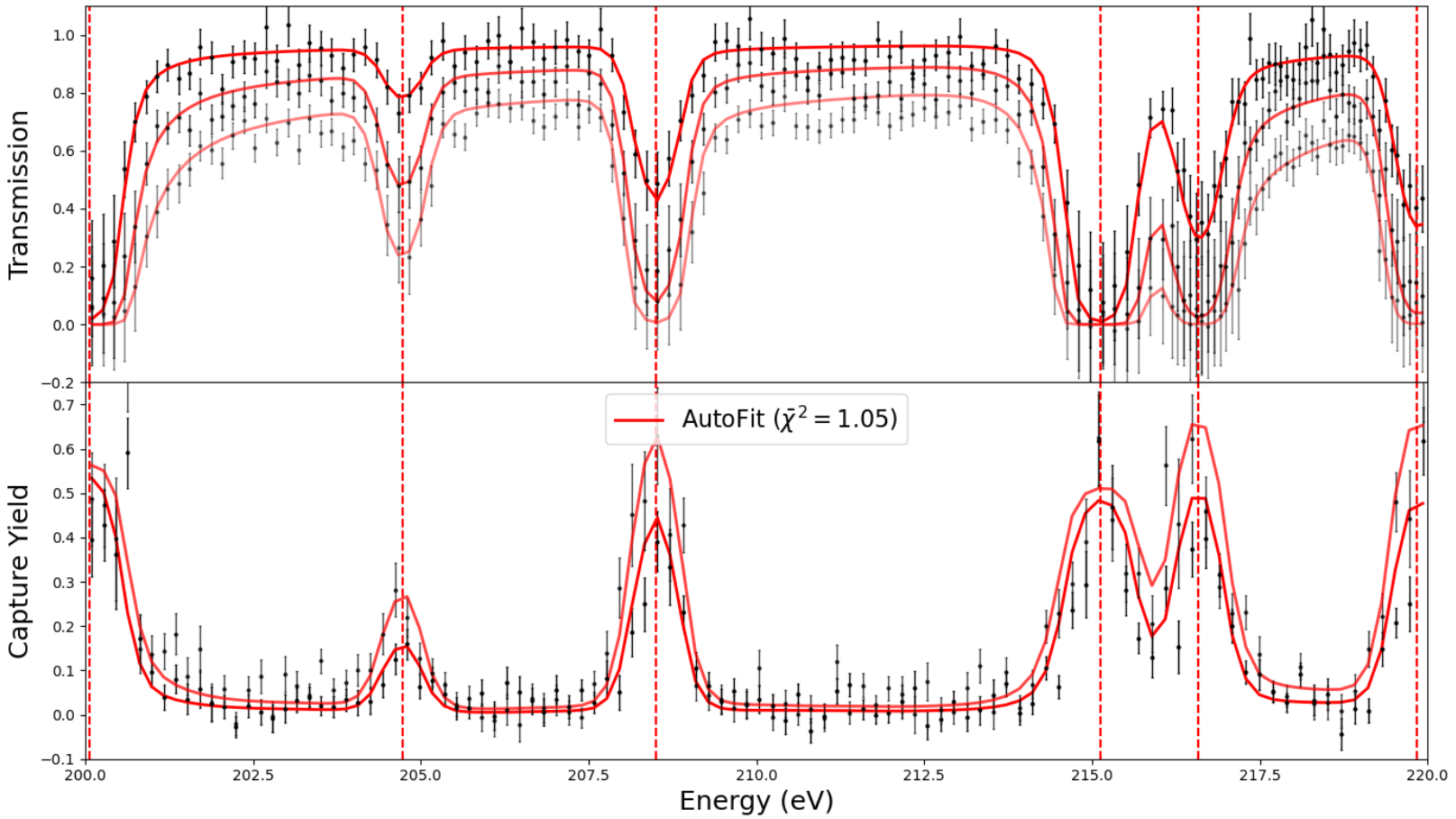
Real Data



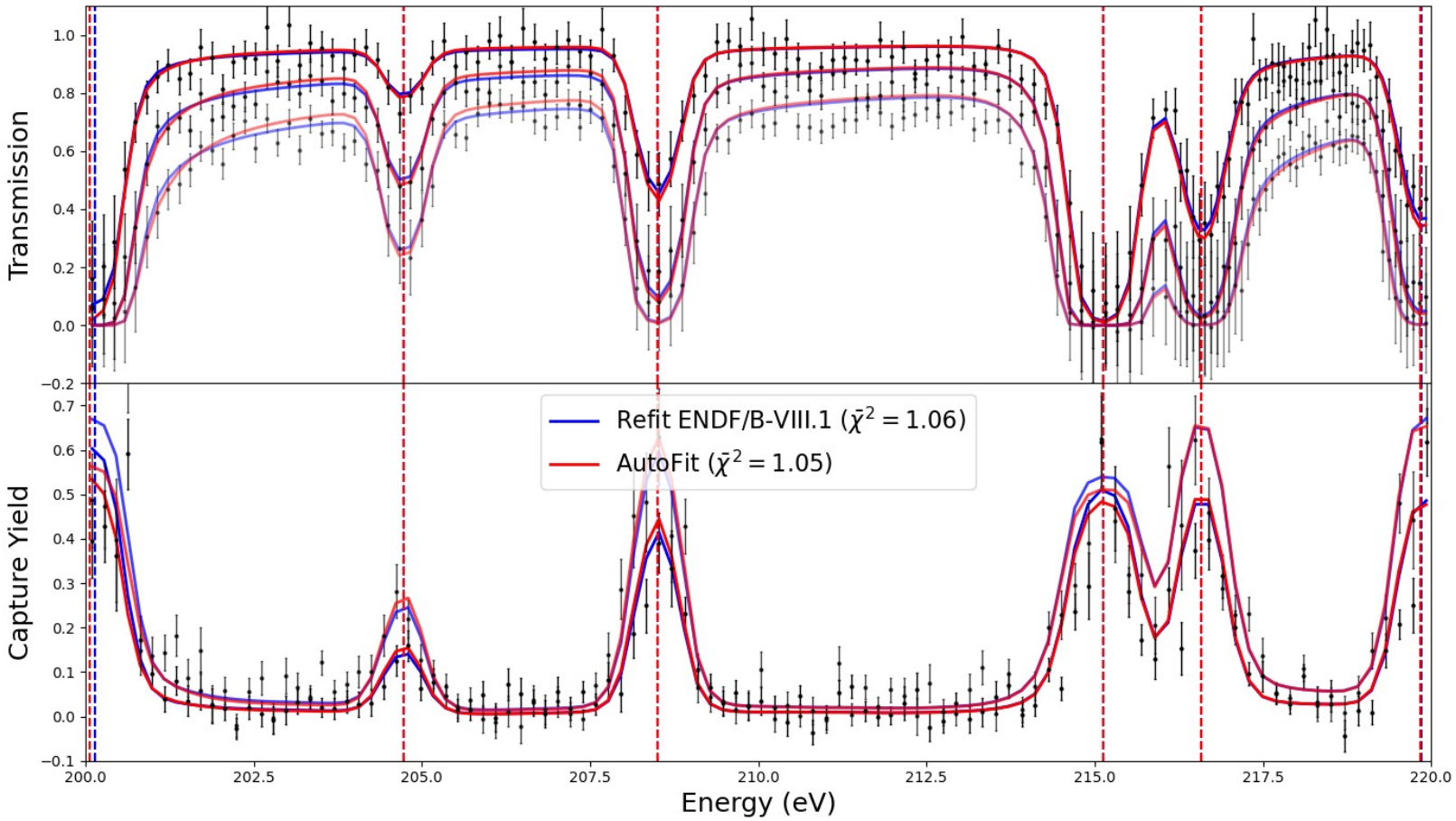
ENDF Fit



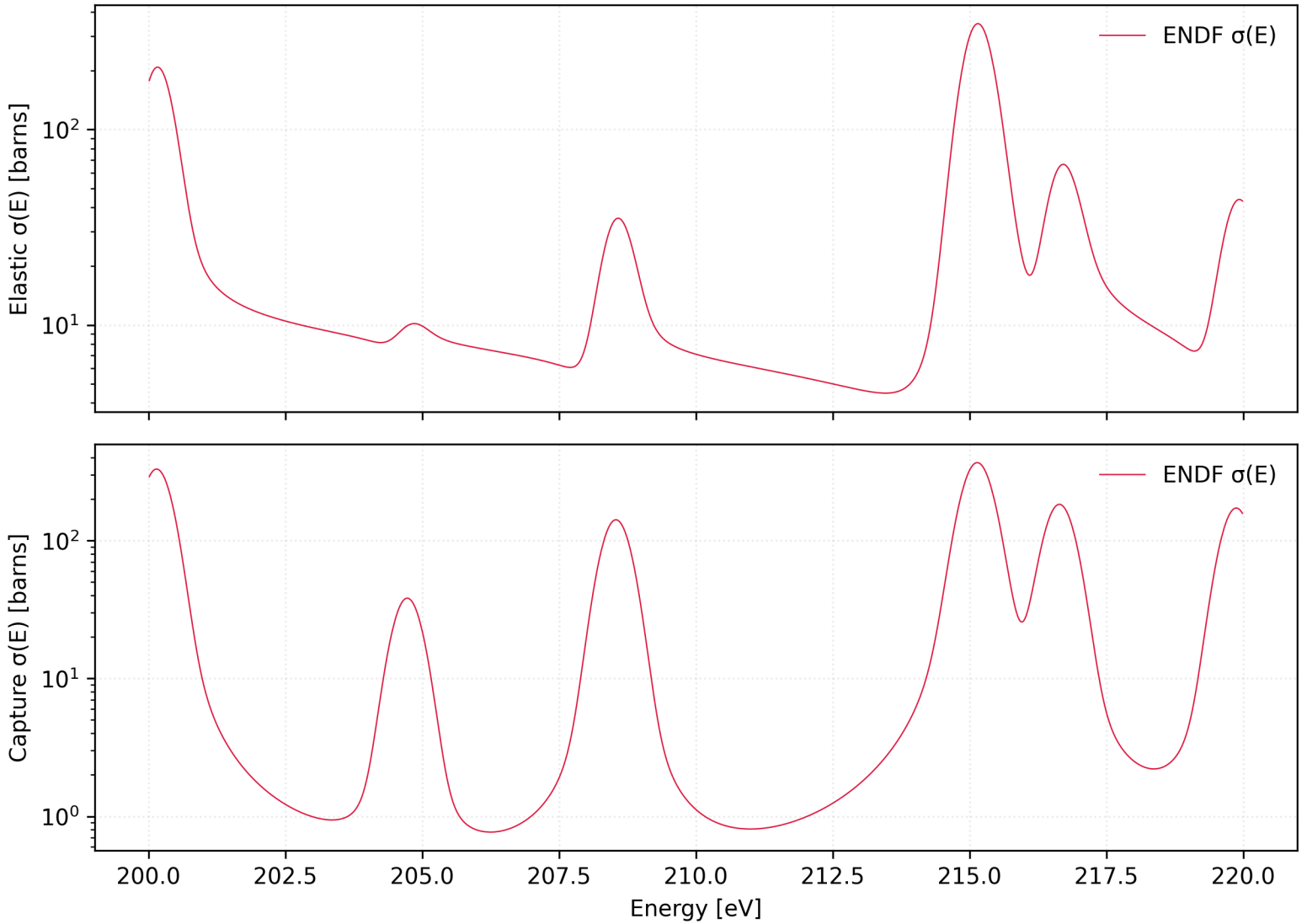
AutoFit



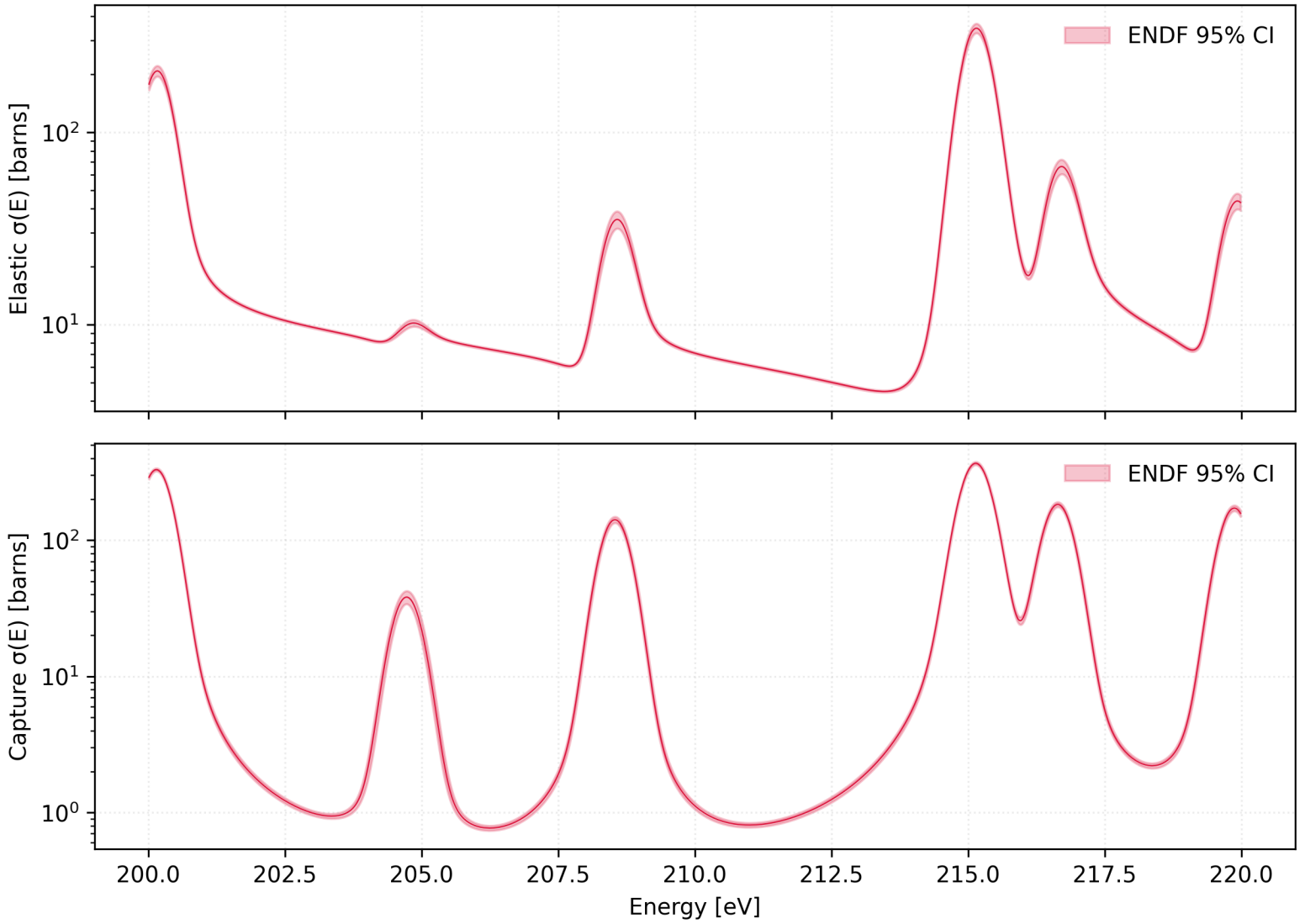
Fit Comparison



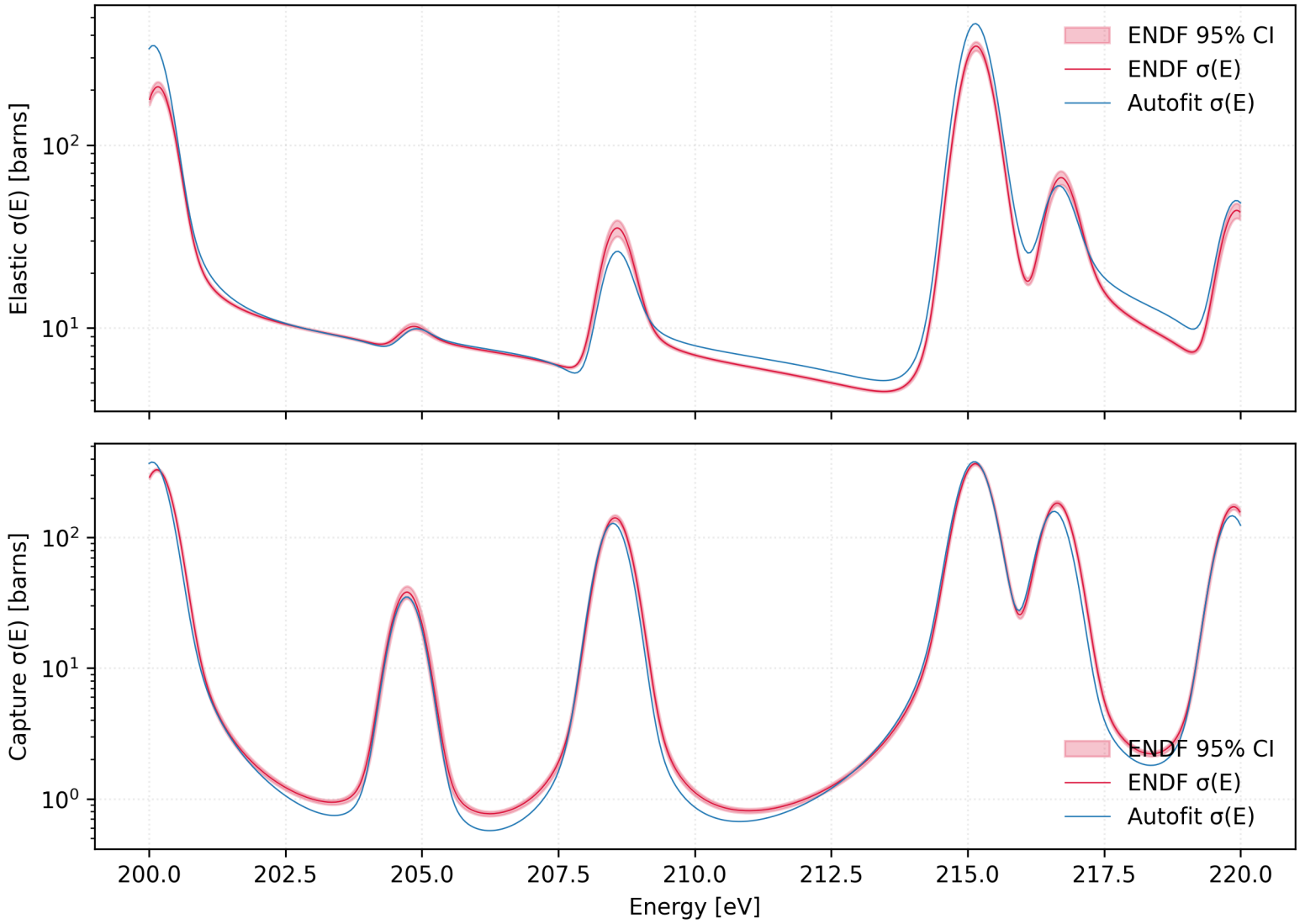
ENDF Cross Section



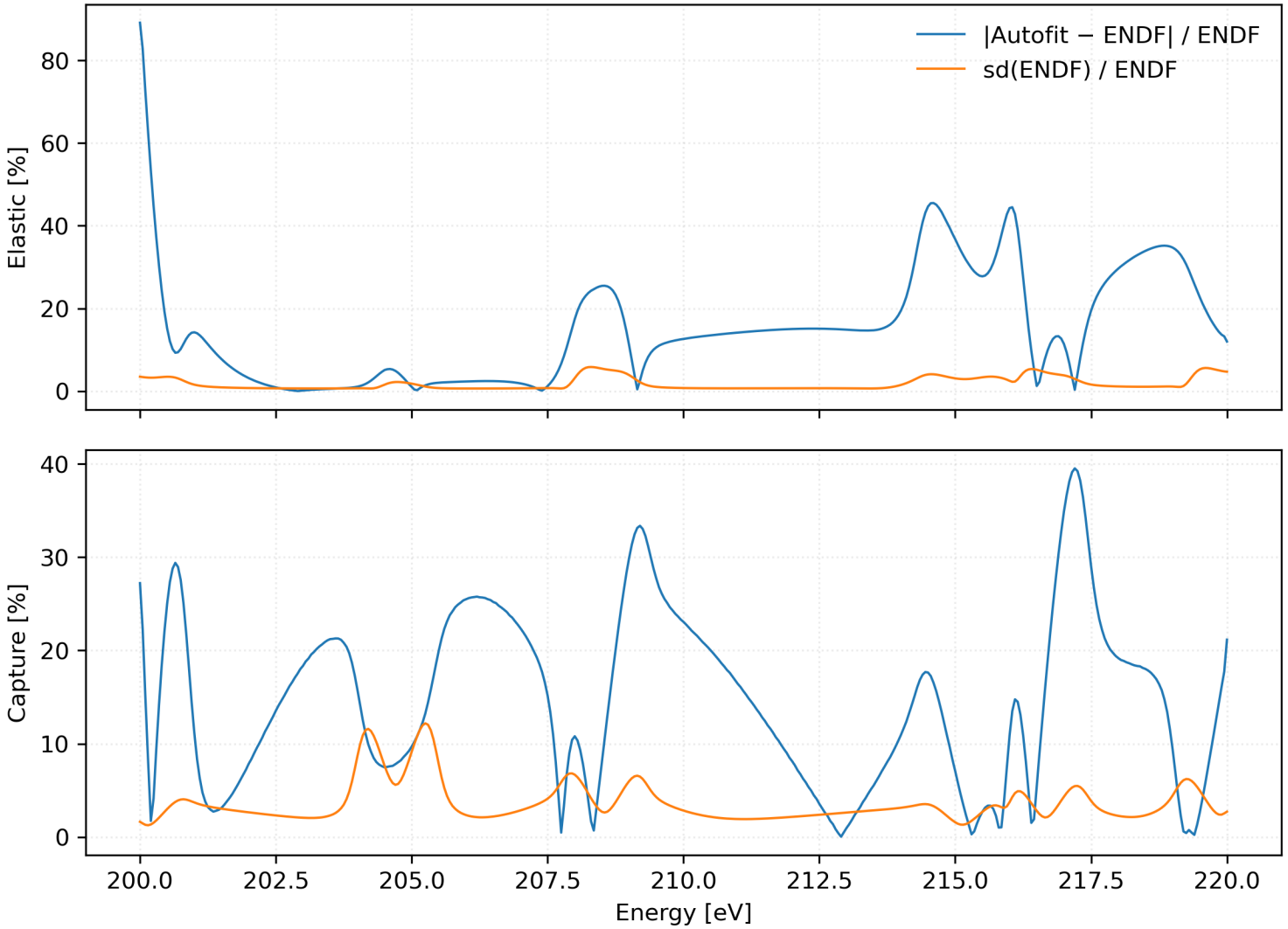
ENDF Confidence Intervals



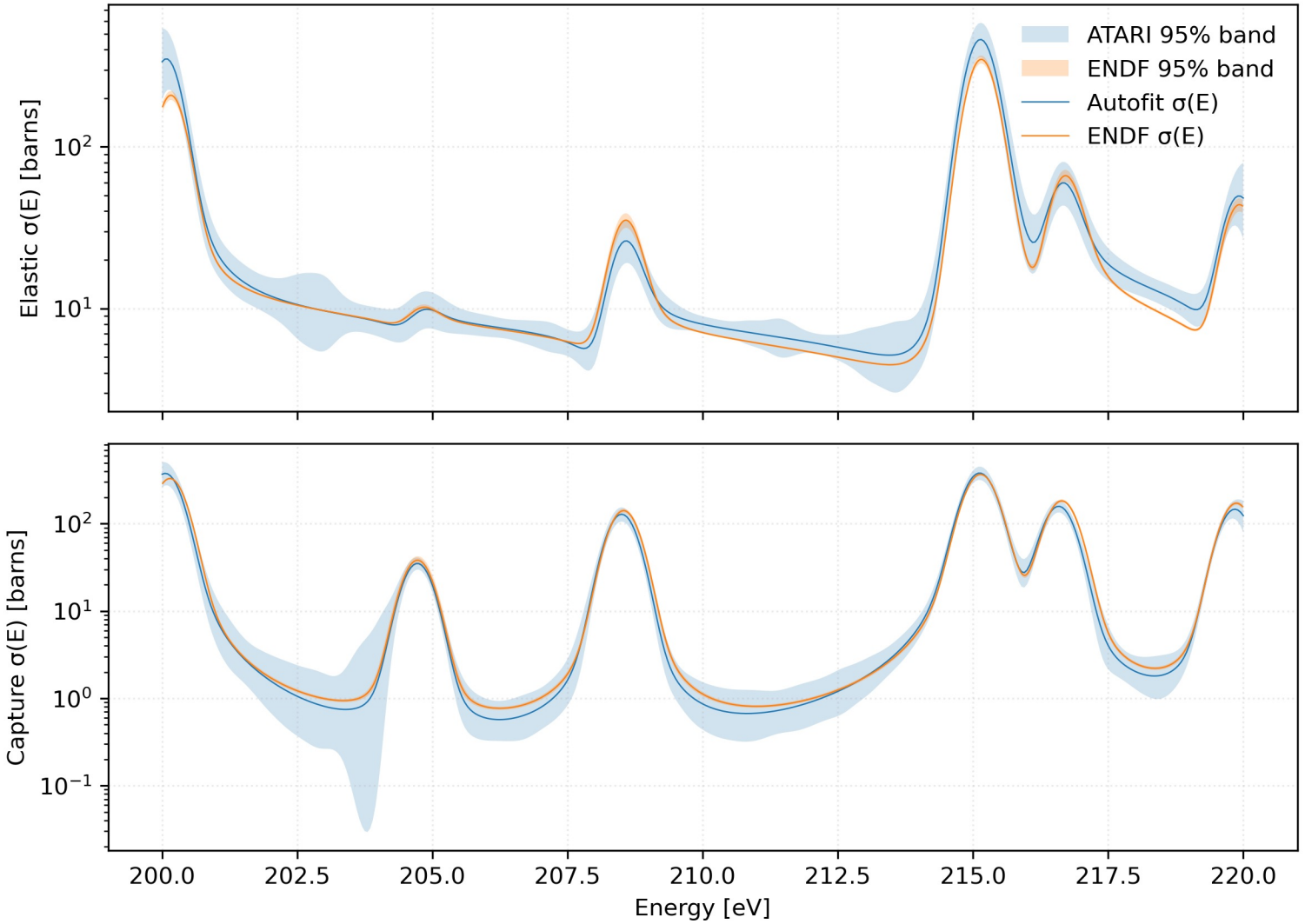
Confidence Intervals vs. Alternate Fit



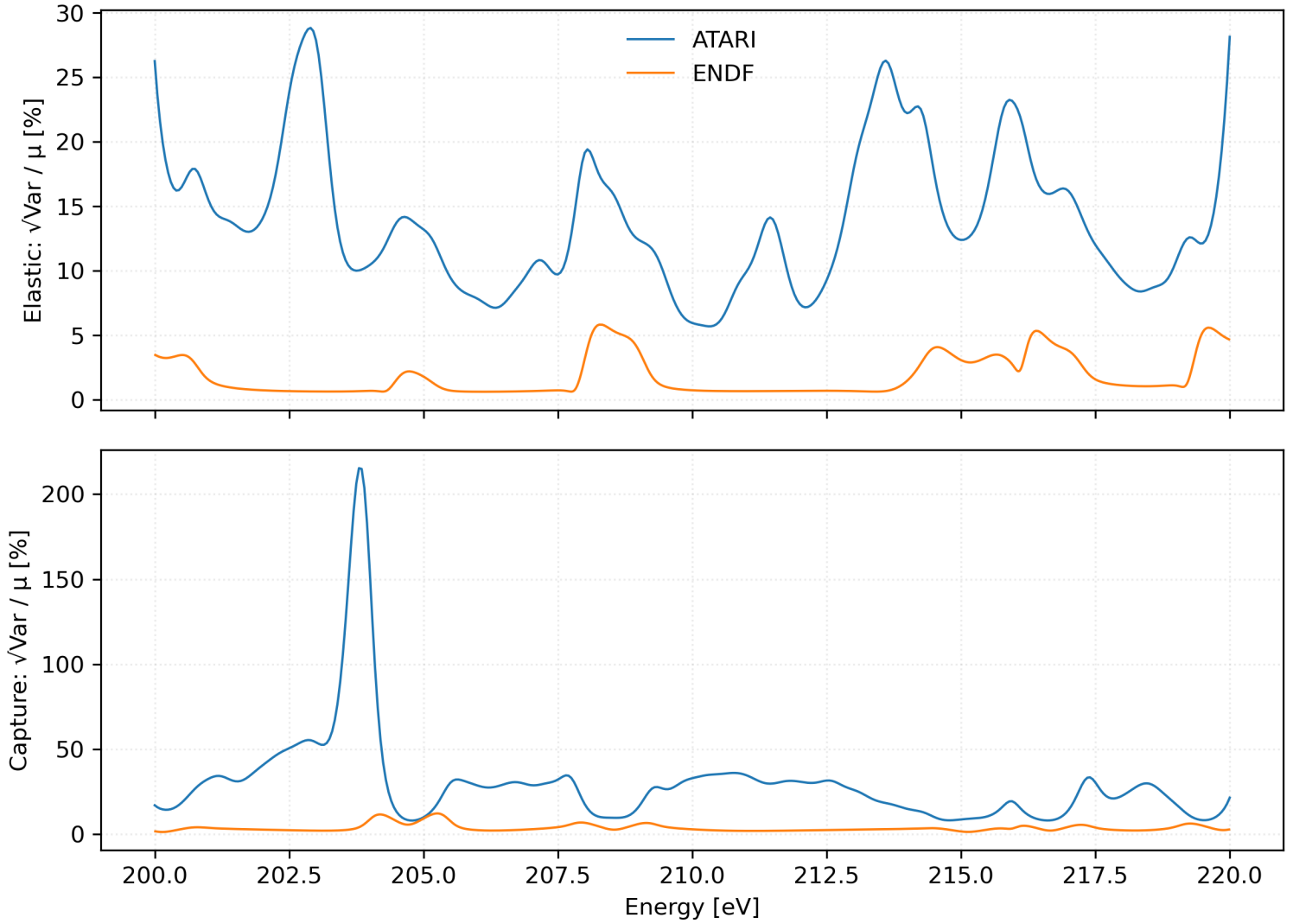
Confidence Intervals vs Relative Difference



AutoFit Confidence Intervals



AutoFit Confidence Intervals

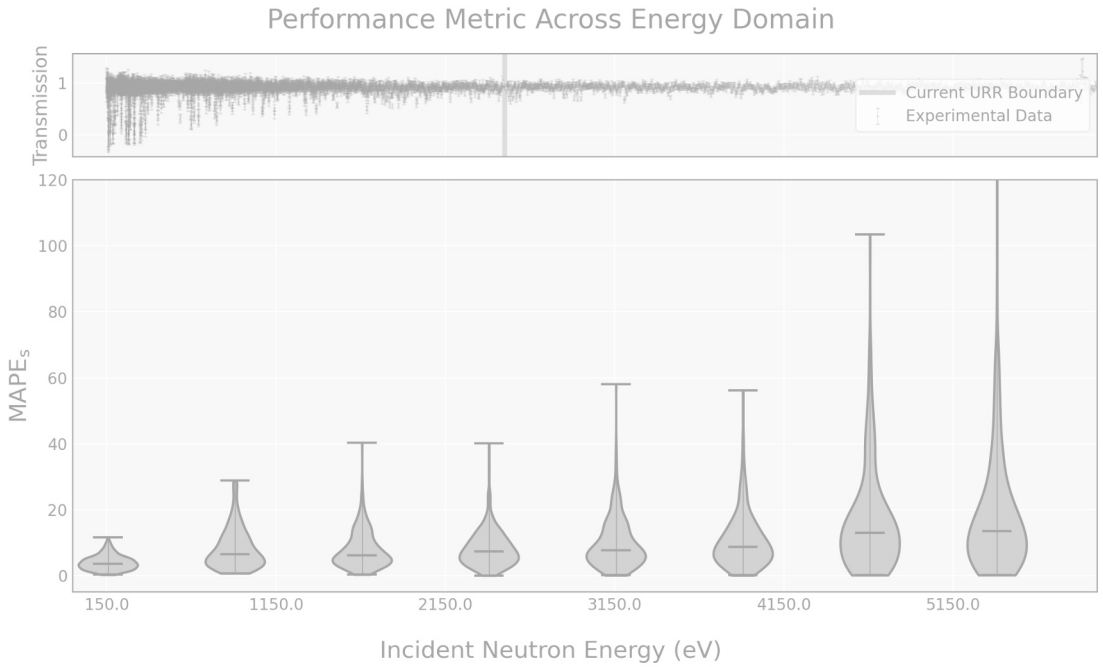


Summary

1. Can estimate the actual cross section inference uncertainty using high-fidelity synthetic data
2. Can (ML-) learn to predict cross section inference uncertainty reliably
3. Log-normal distribution of error performs best in quantitative testing

Future work

- Expand to full RRR (current test at low-energy)
- Explore other error distributions
- Demonstrate impact of updated uncertainty evaluation on benchmarks/applications



This material is based upon work supported by the Department of Energy National Nuclear Security Administration through the Nuclear Science and Security Consortium under Award Number(s) DE-NA0003996.

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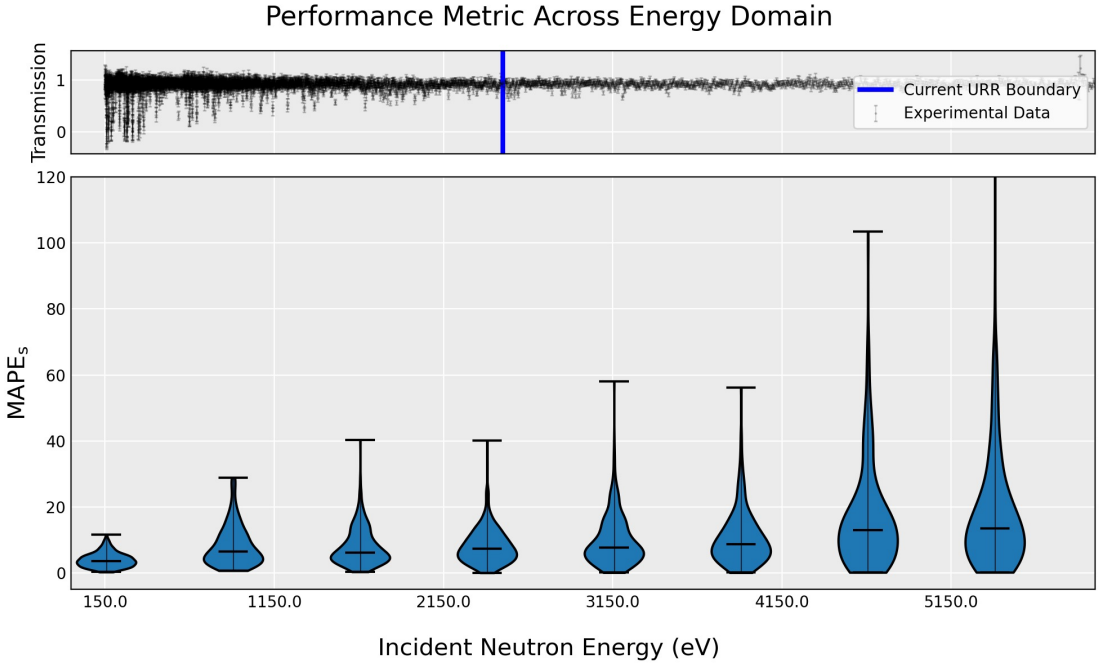

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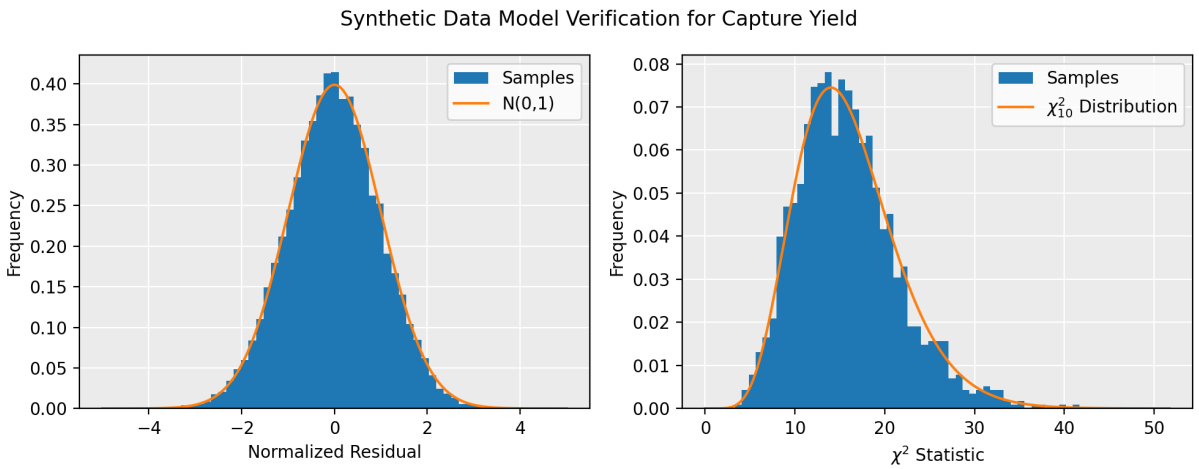
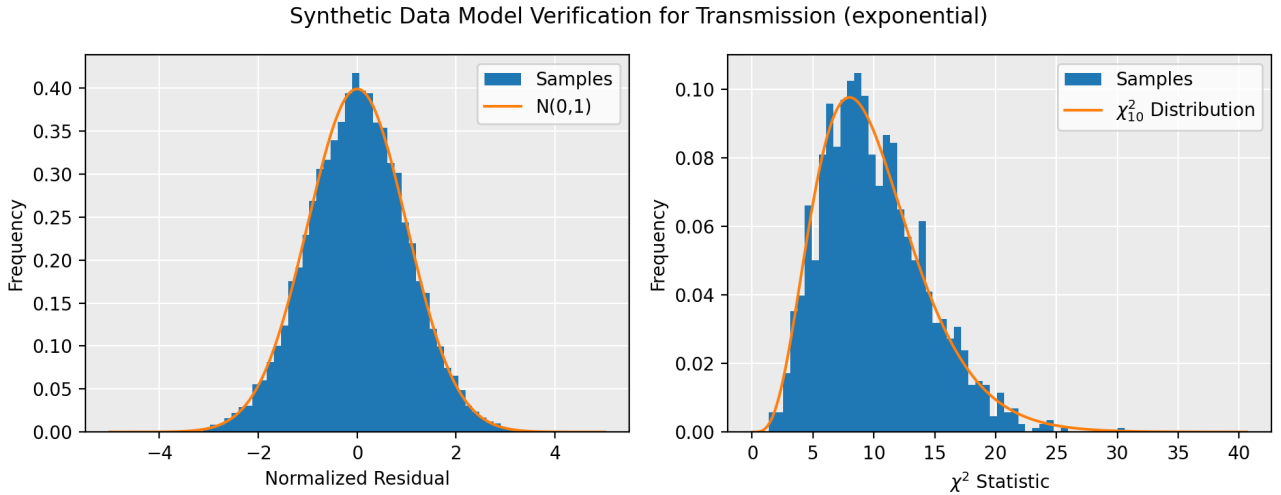
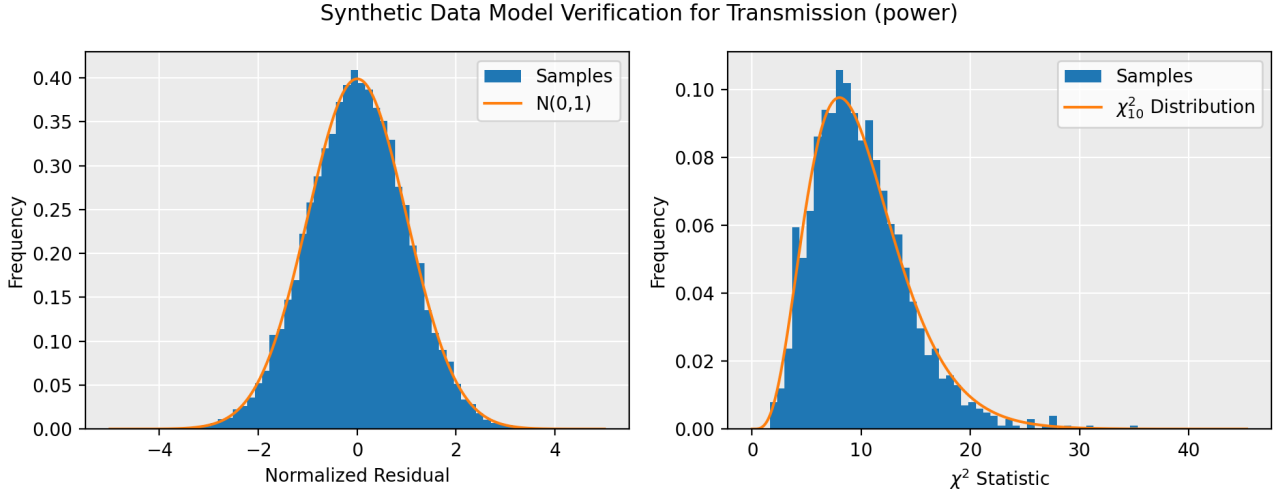
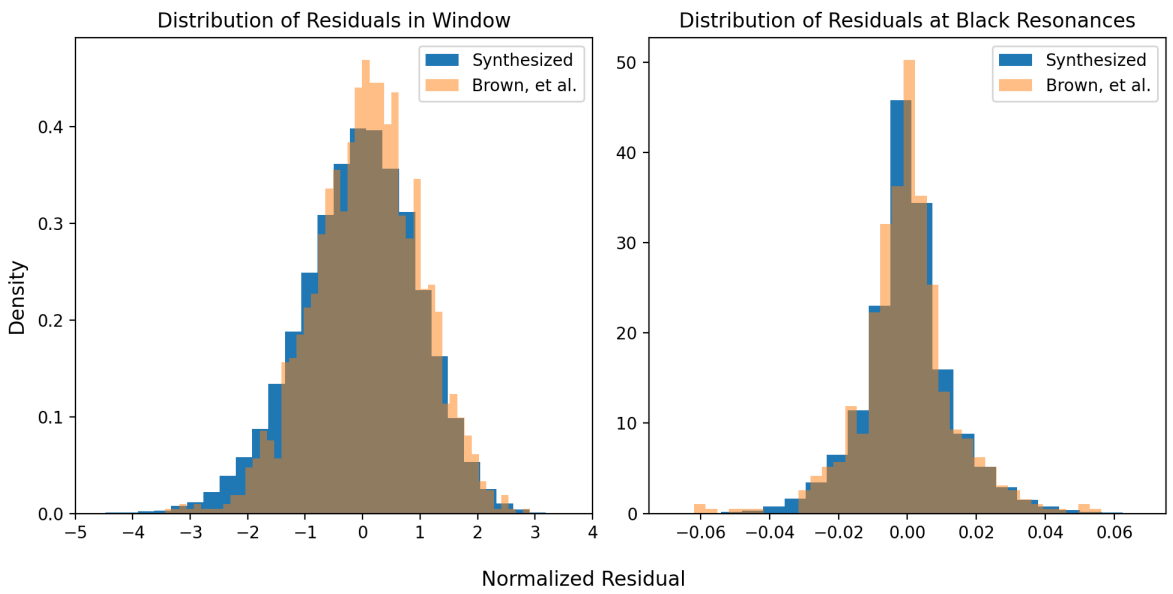
Backup Slides

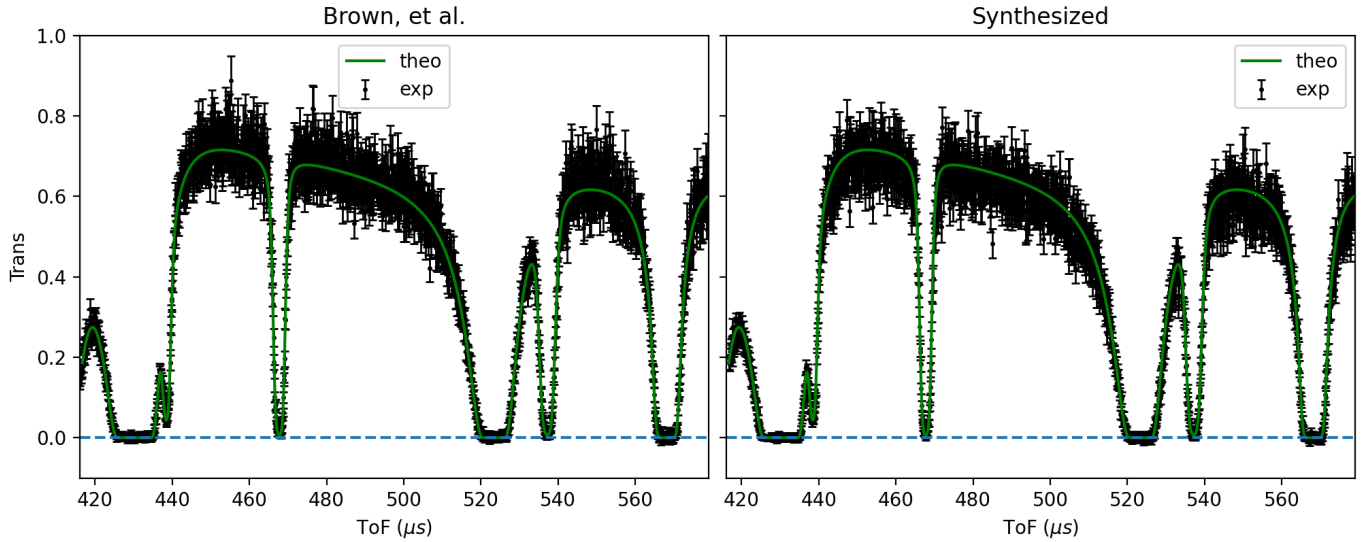
Synthetic Data V & V

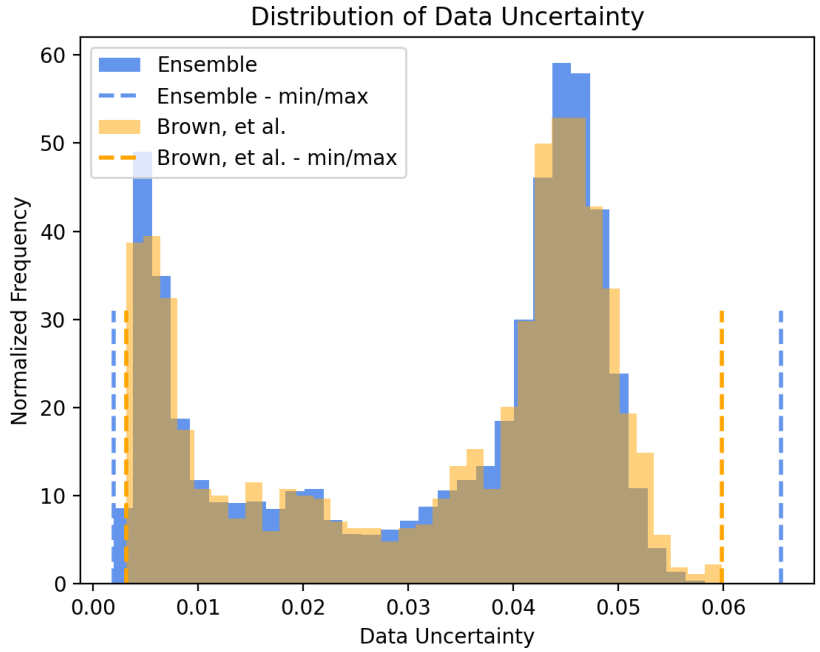


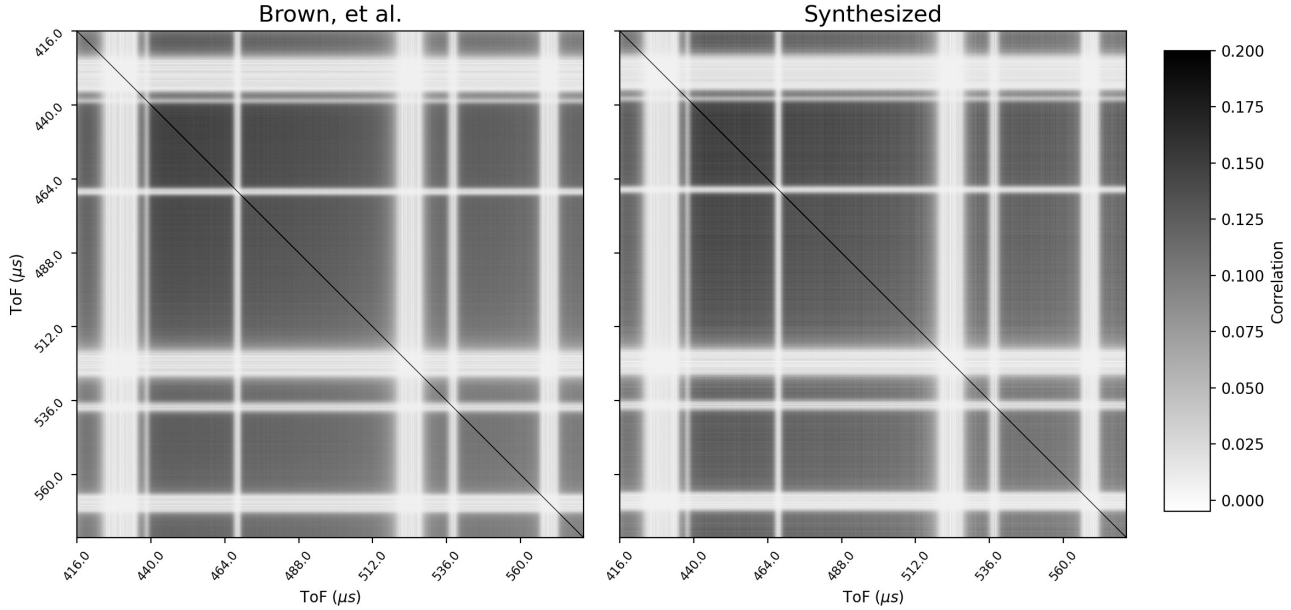


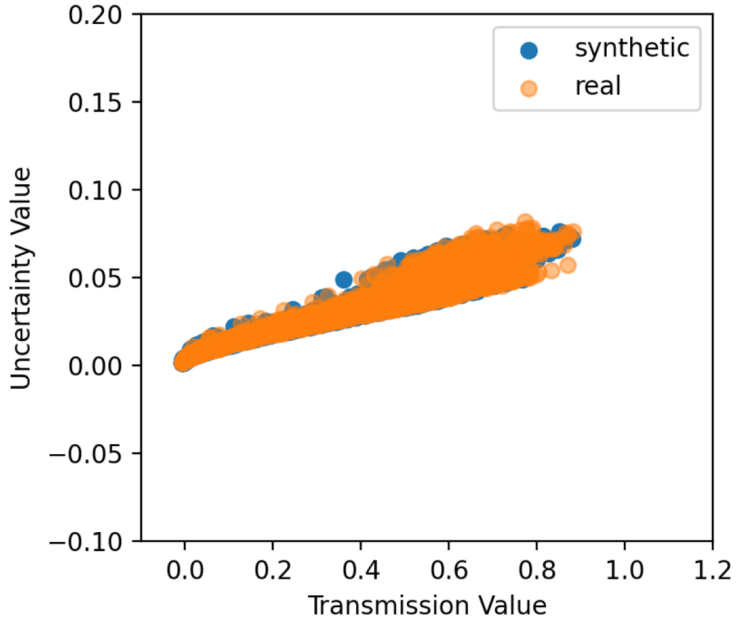


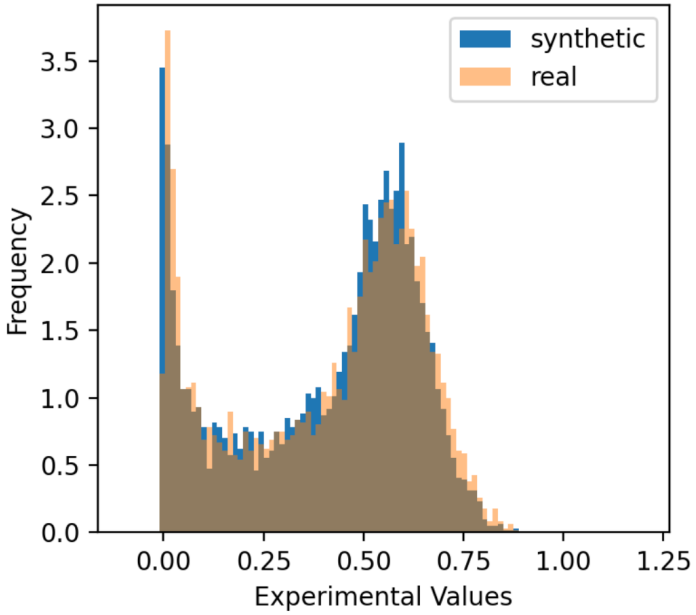


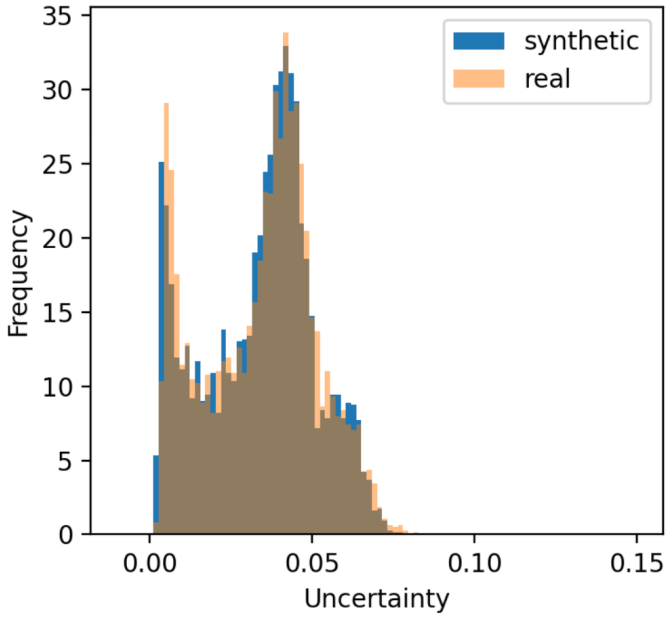


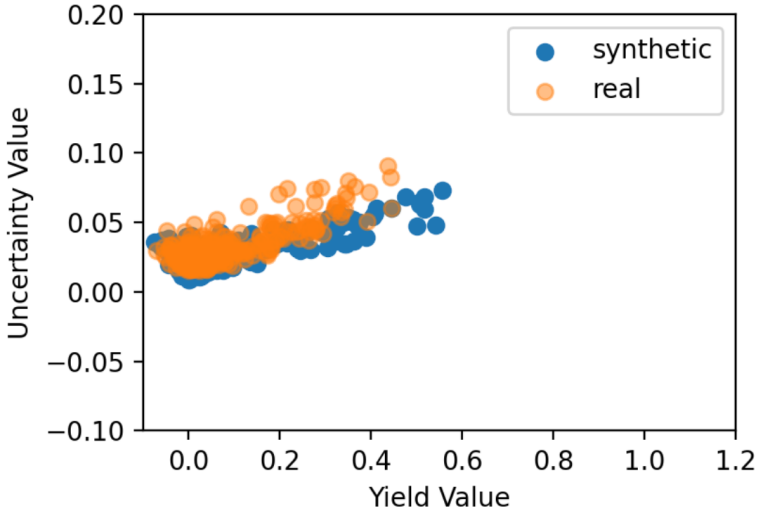


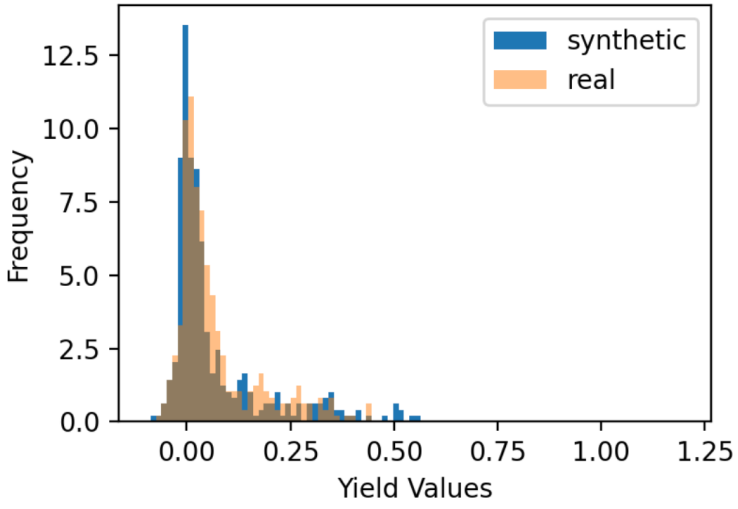


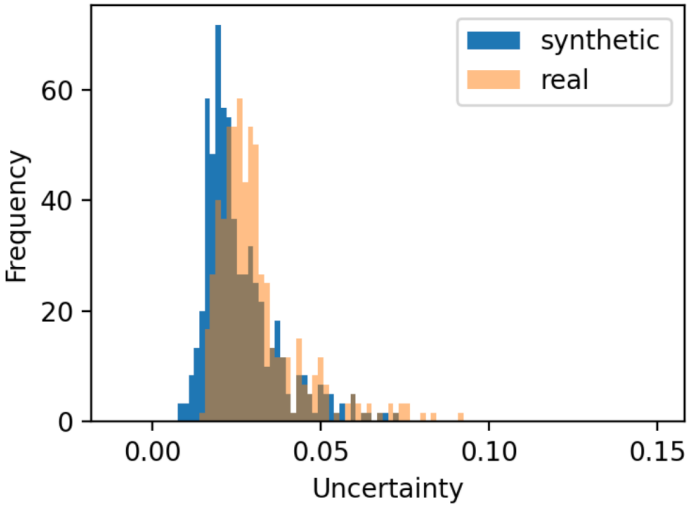




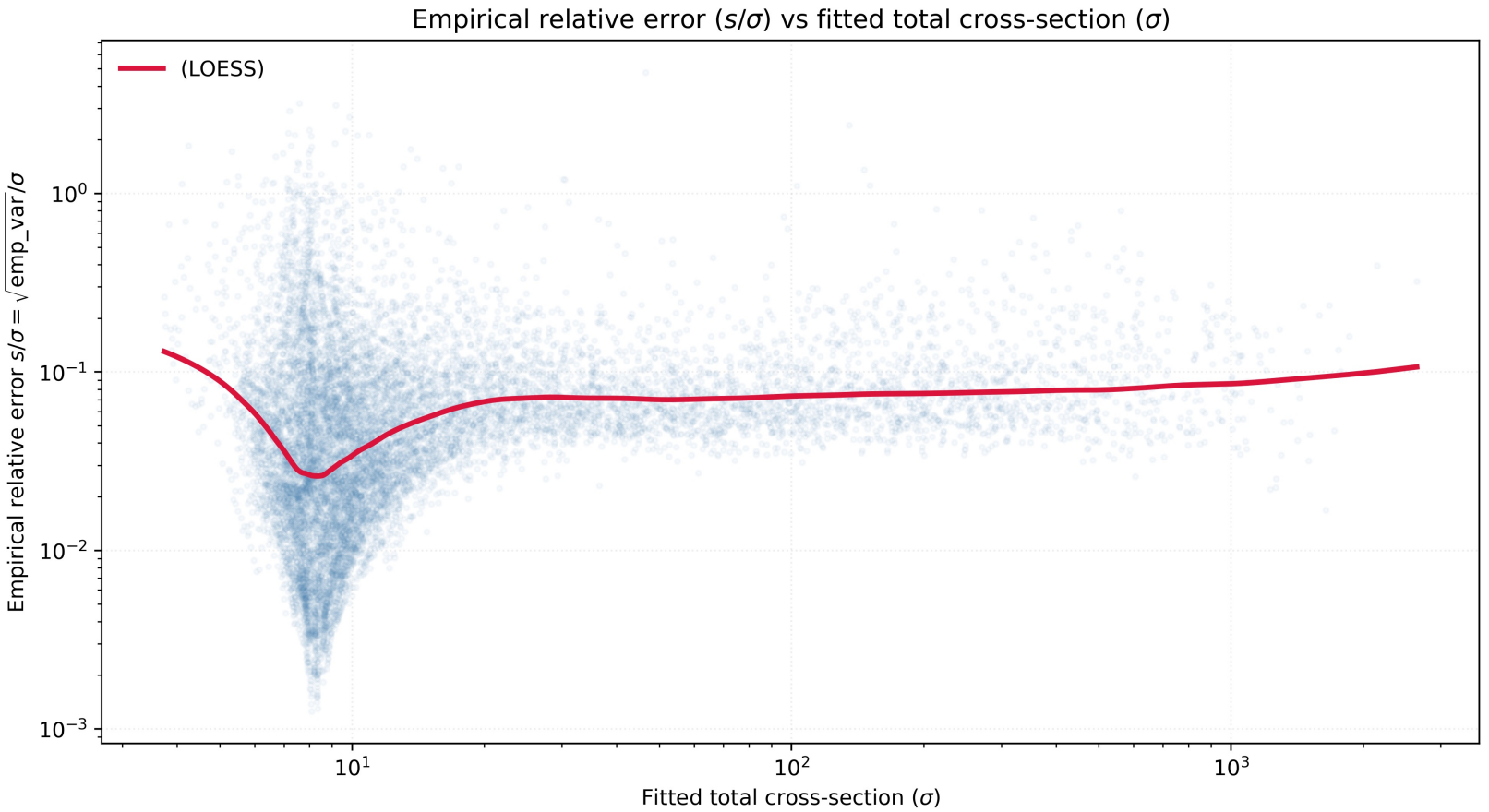




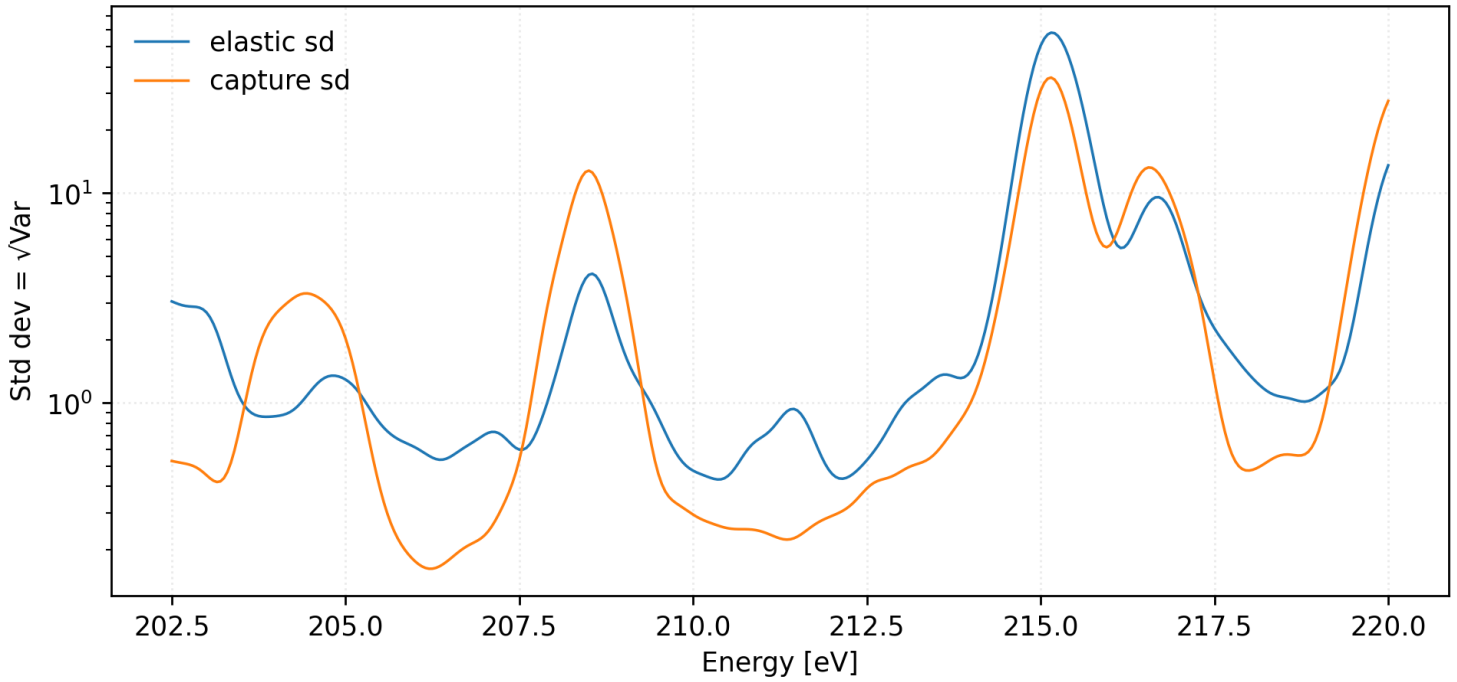




Total Cross Section Error



AutoFit Reaction Relative Error



Distribution of Error

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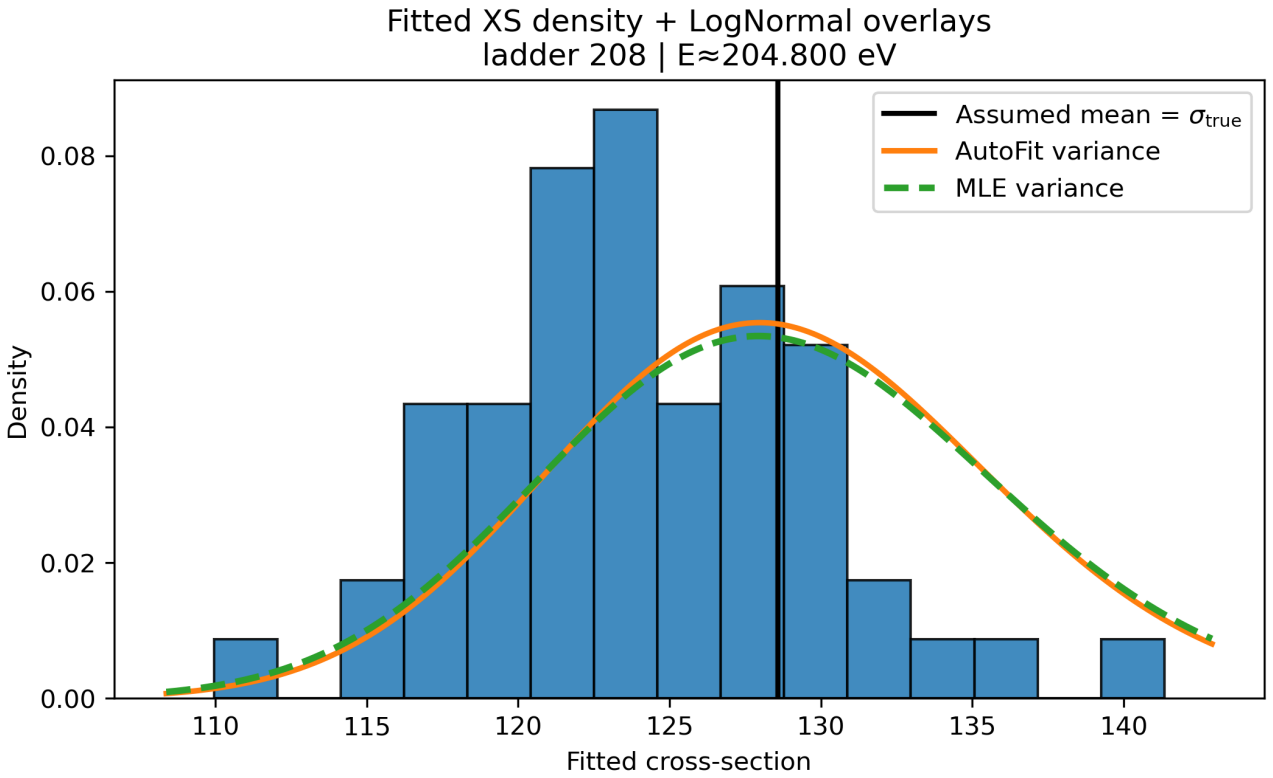

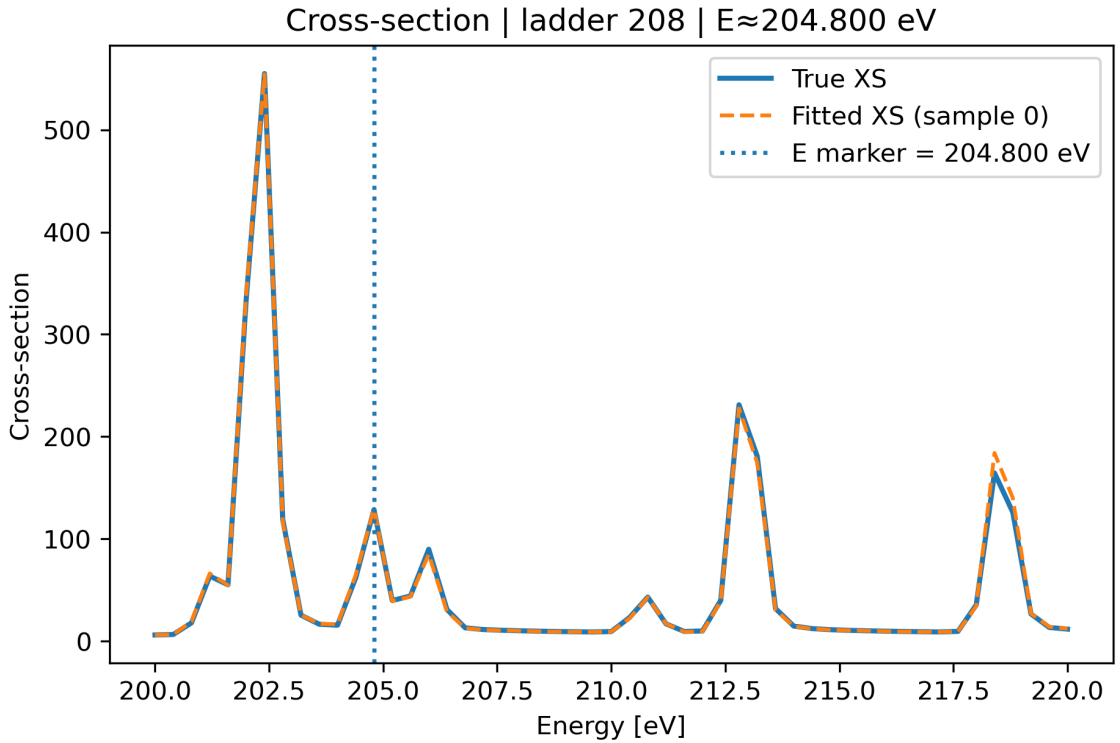

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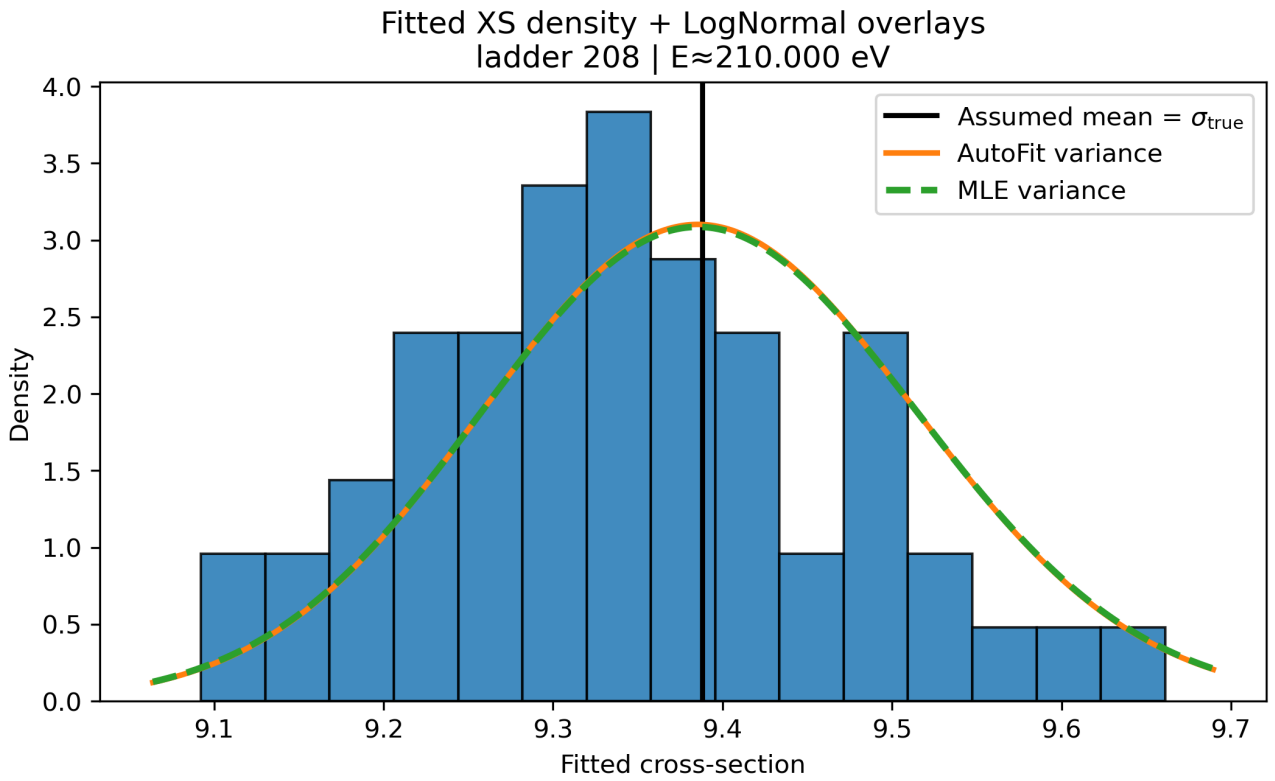

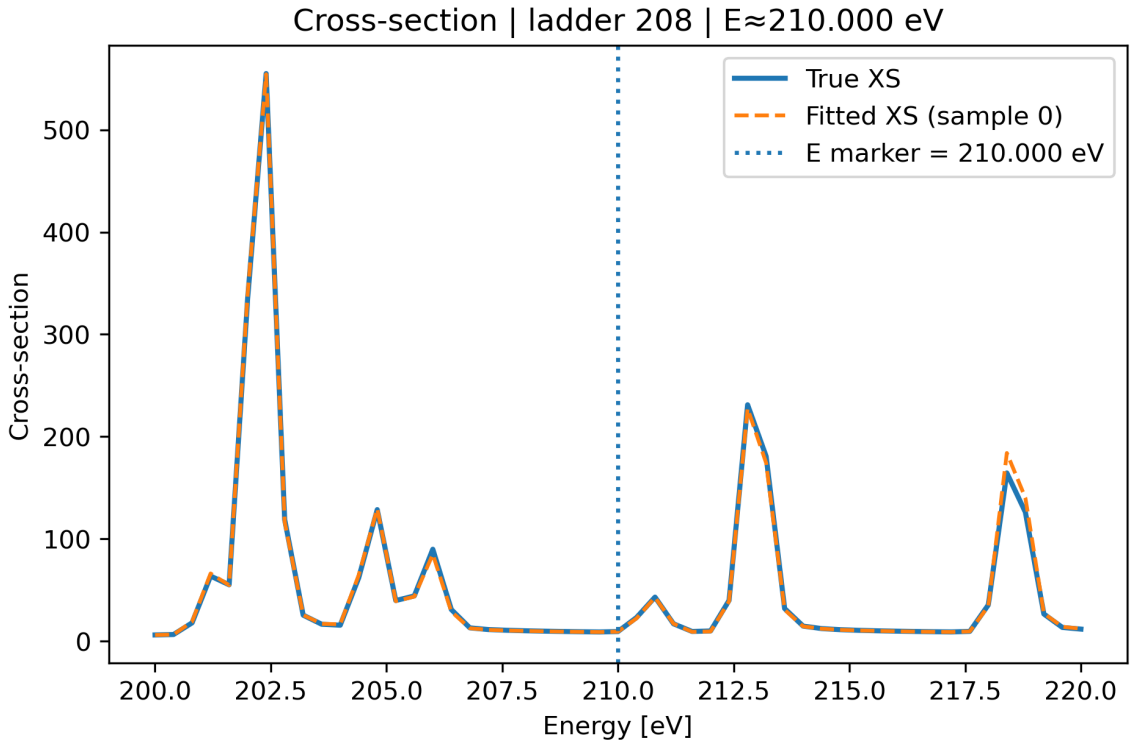

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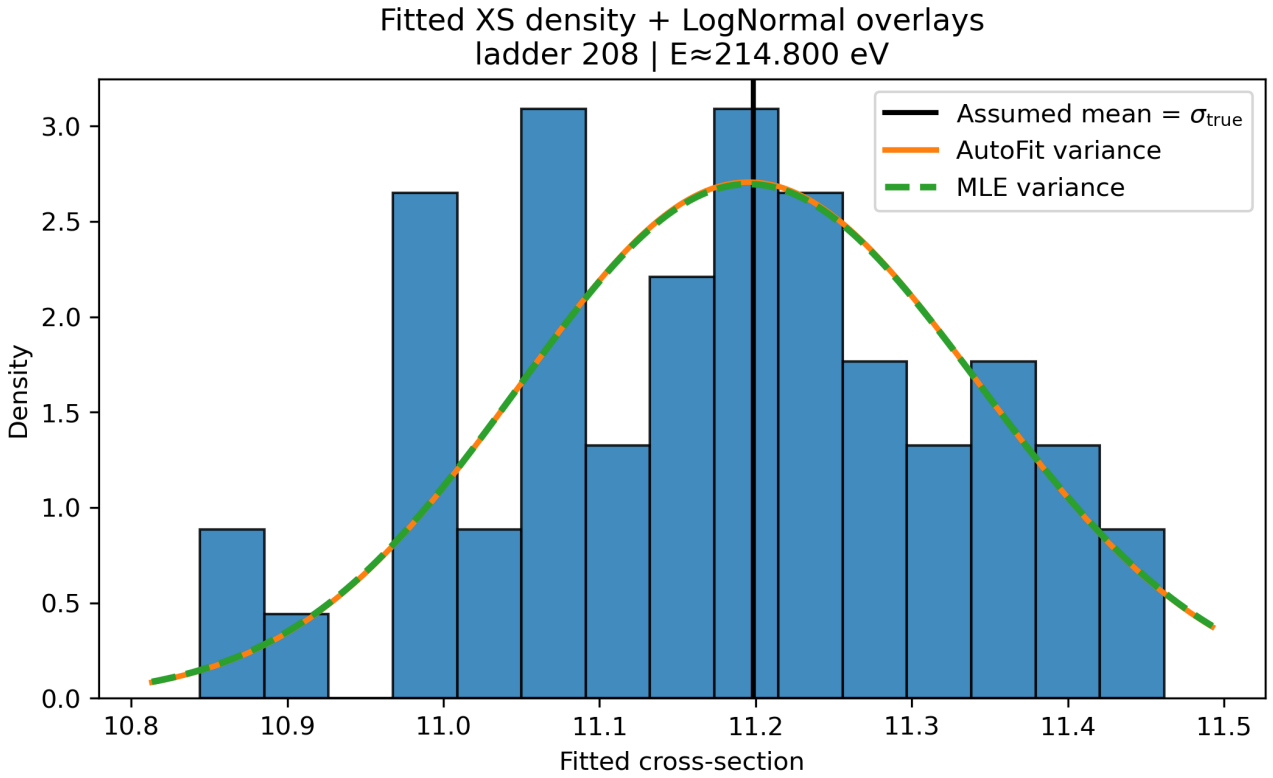

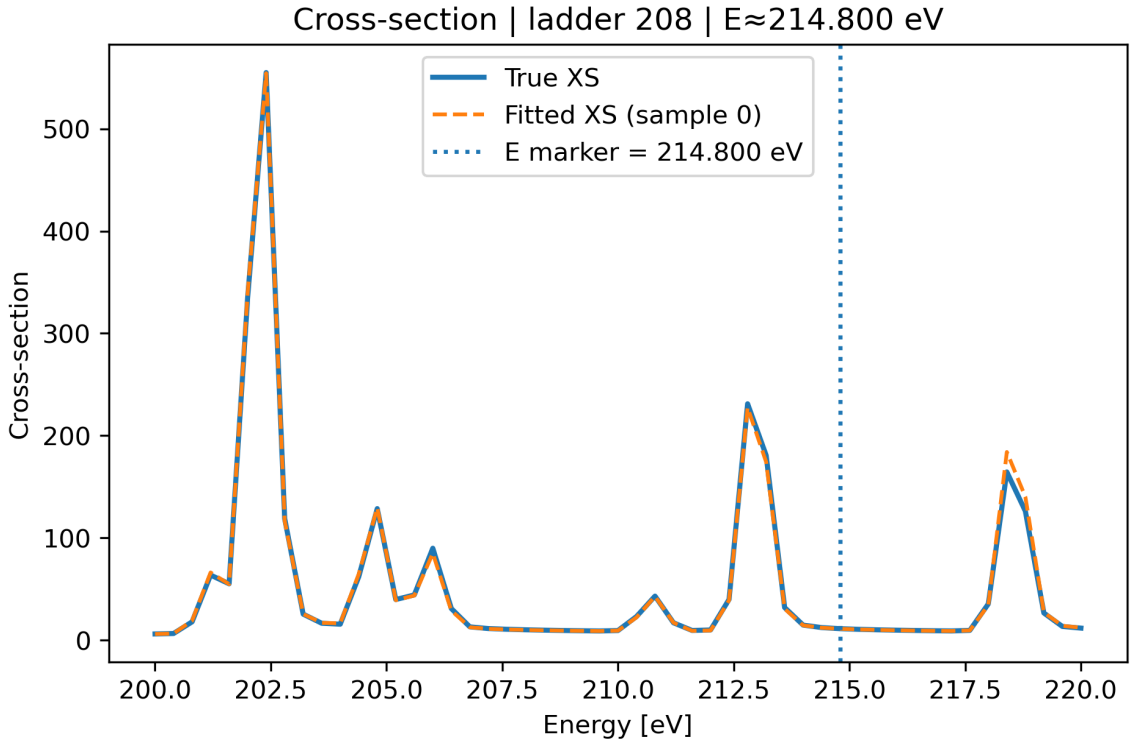

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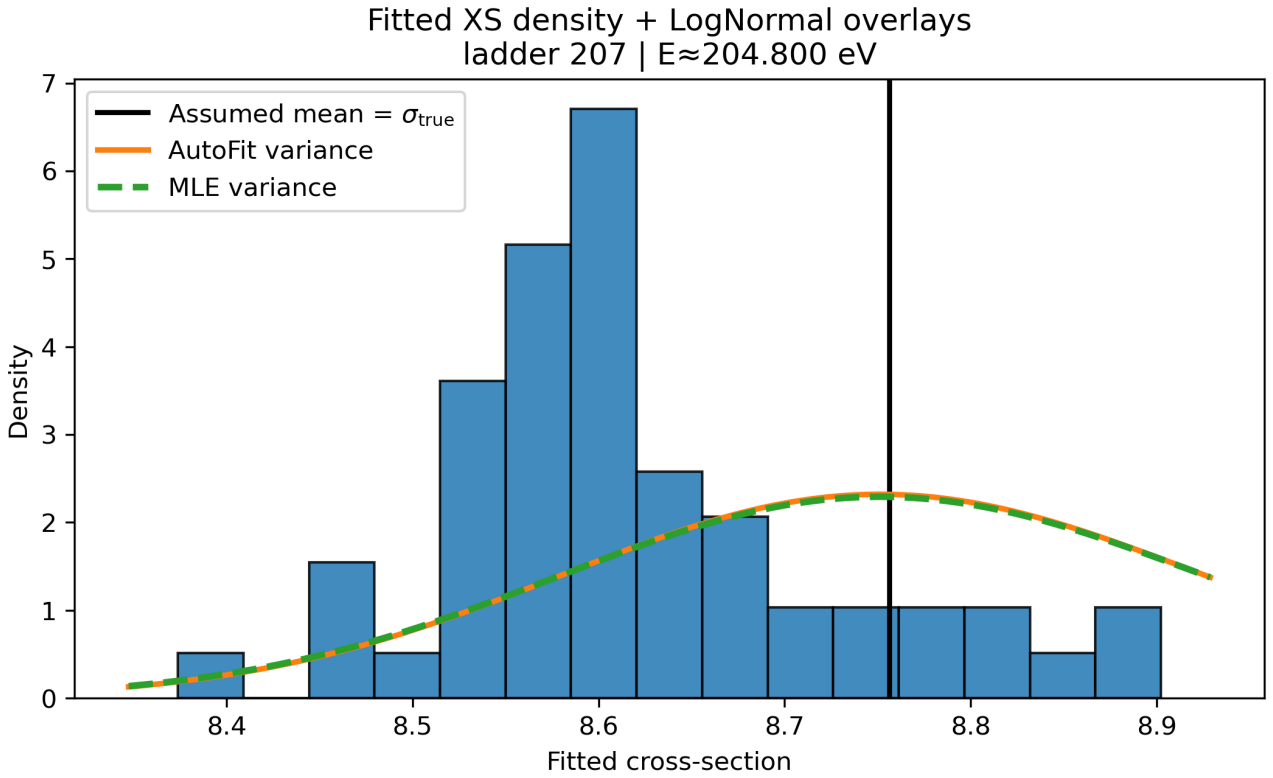

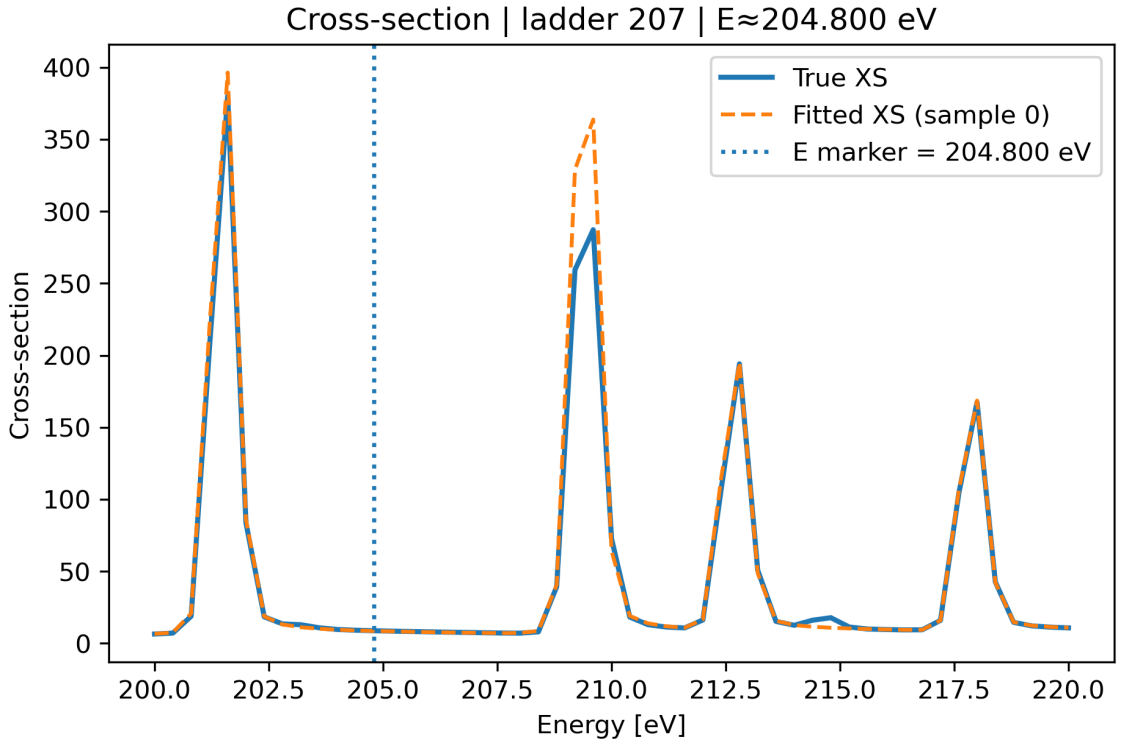

Distribution of Error

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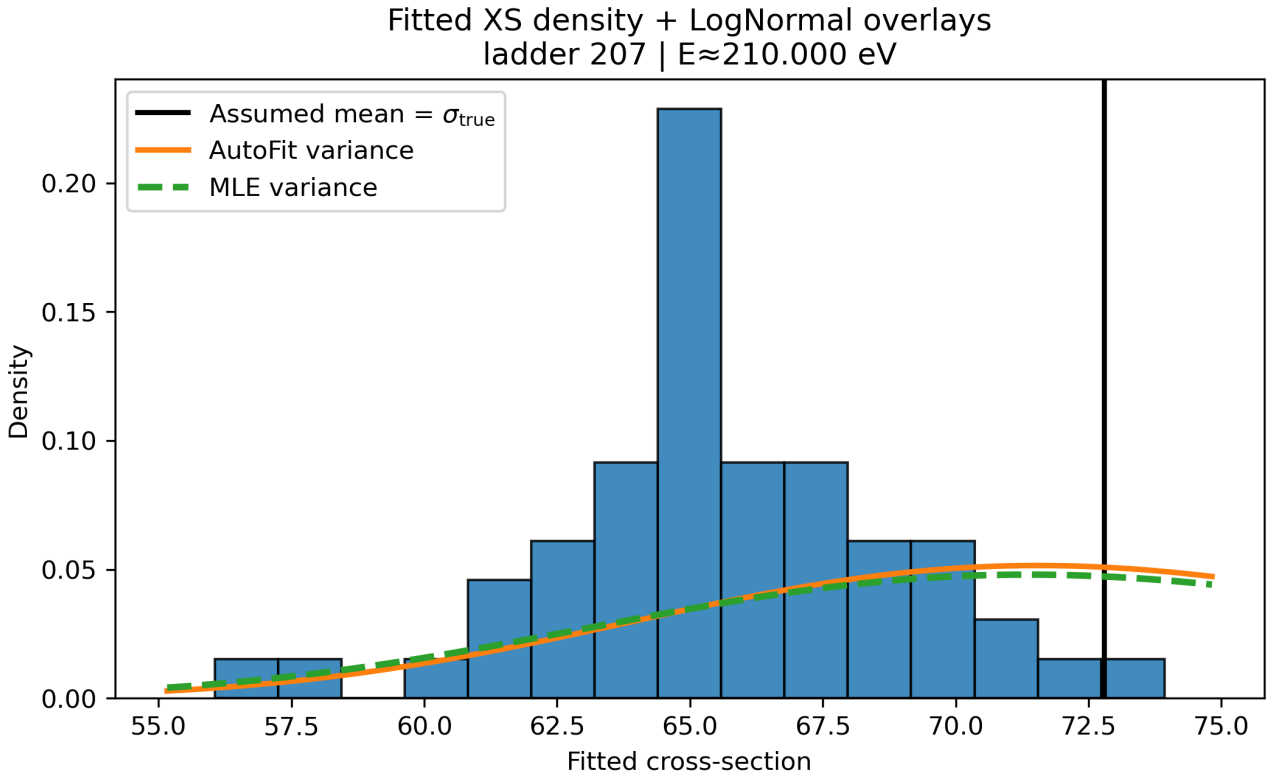

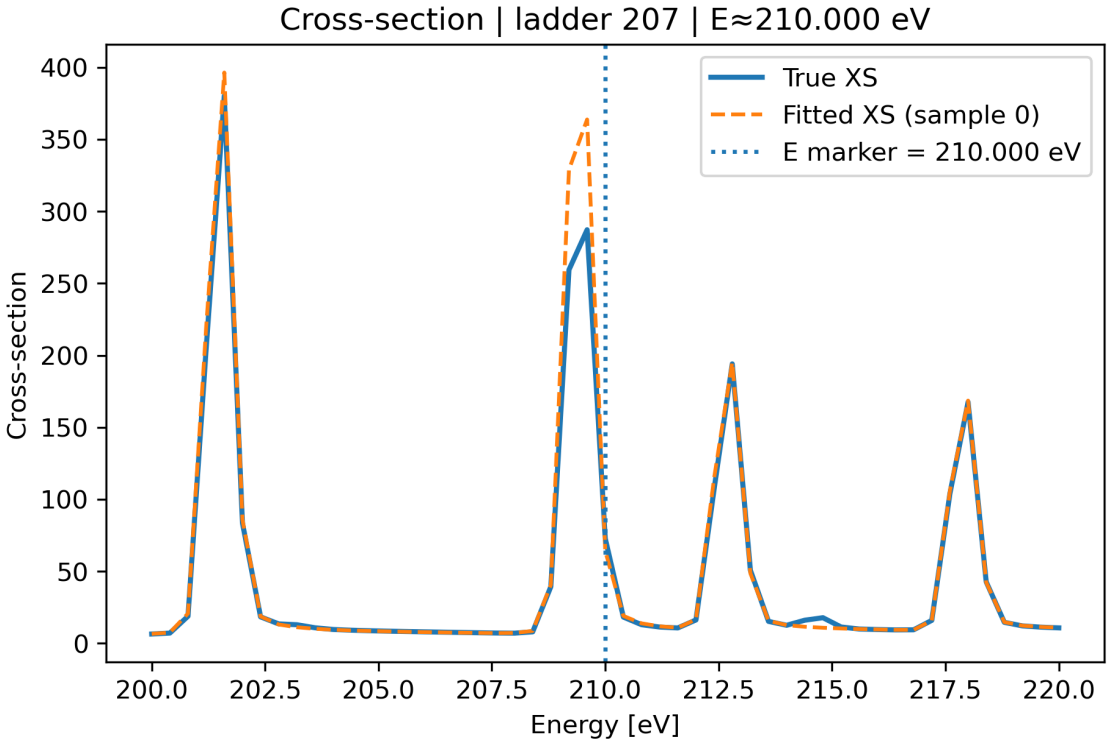

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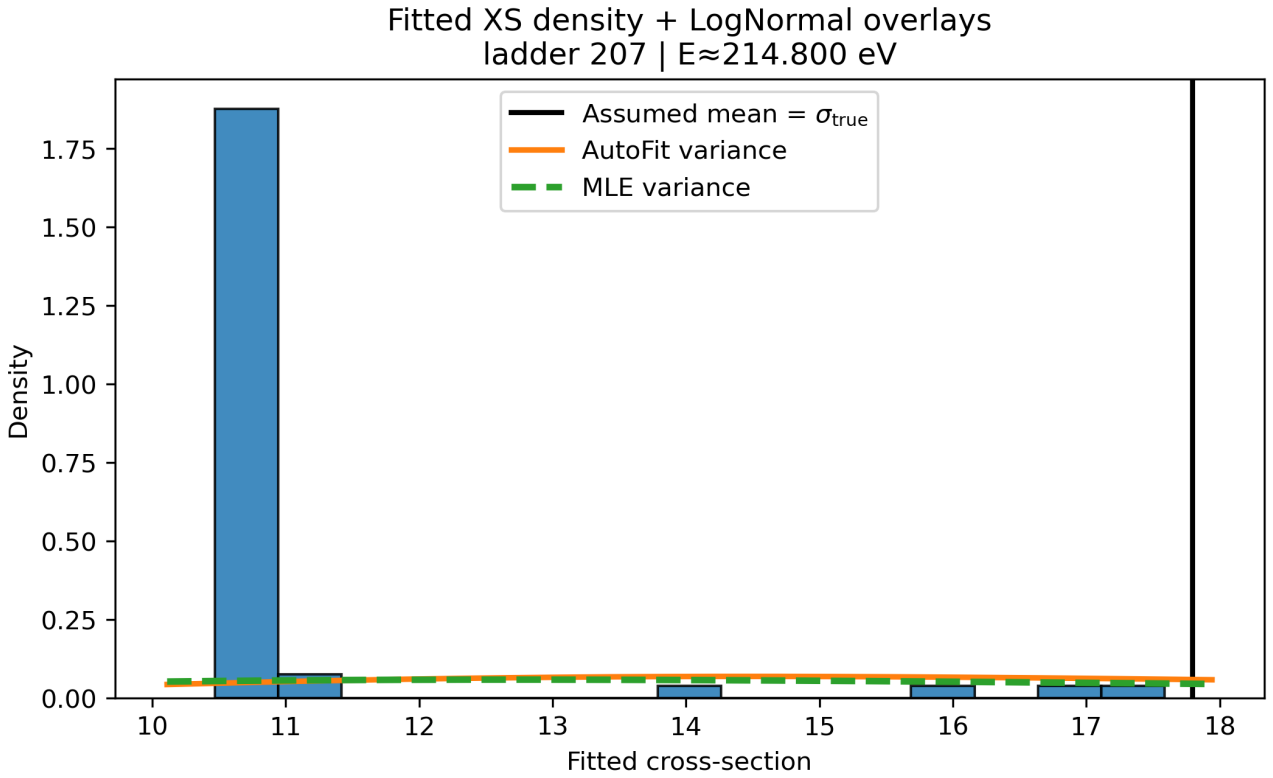
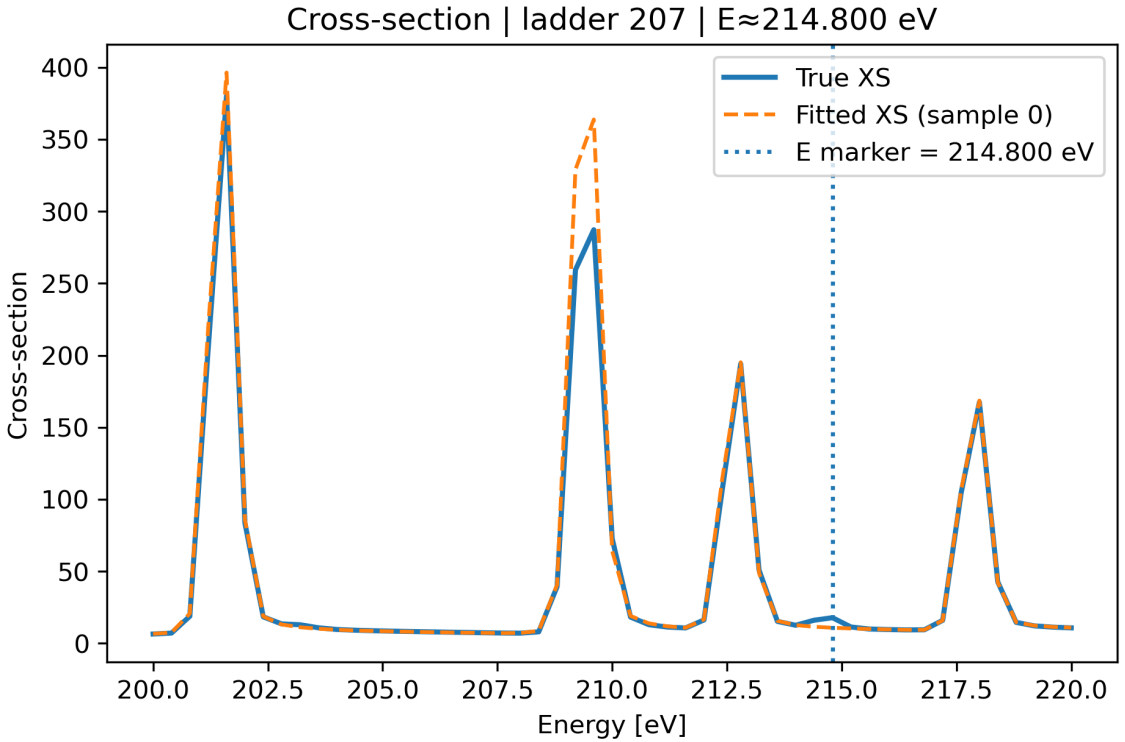
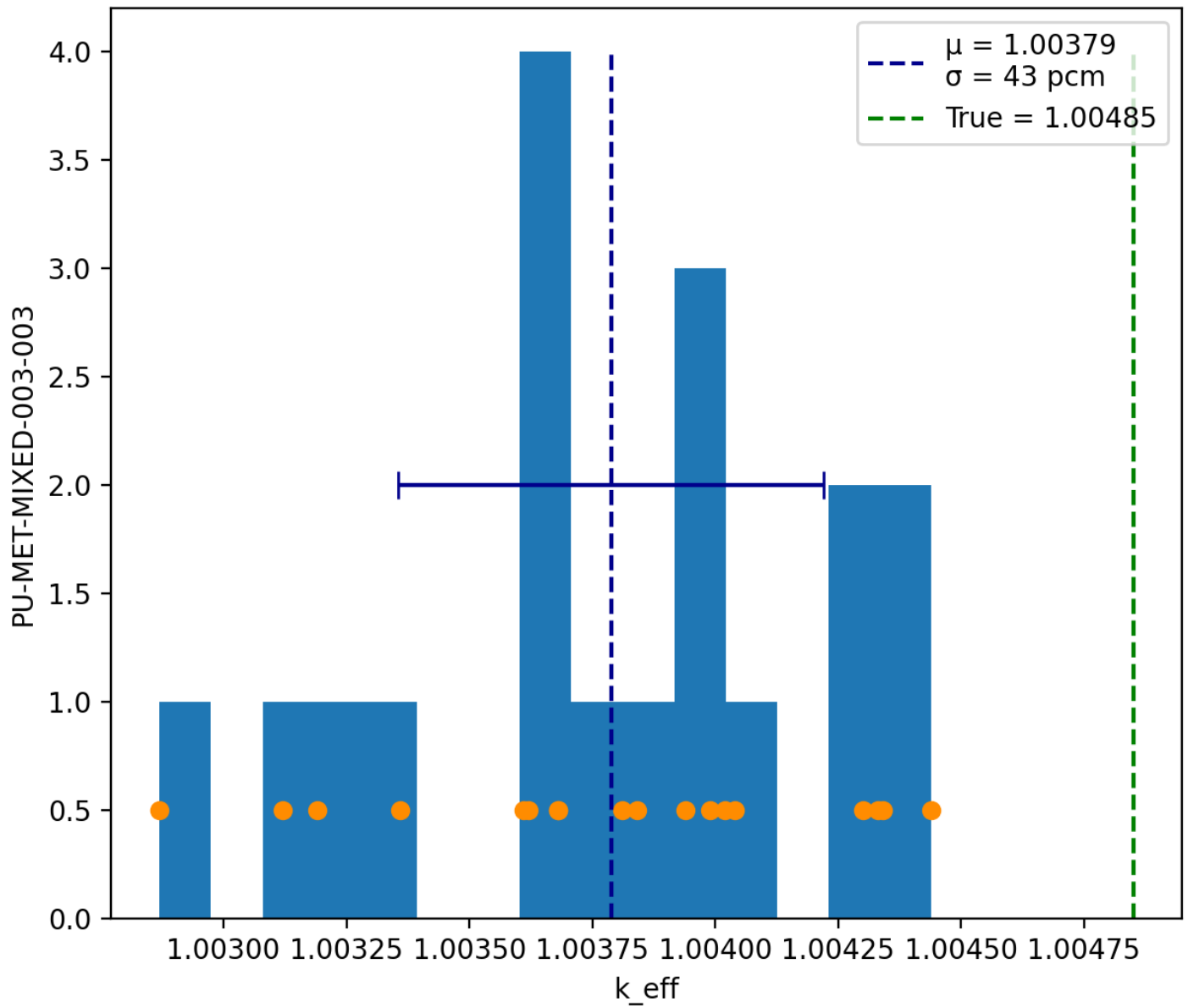
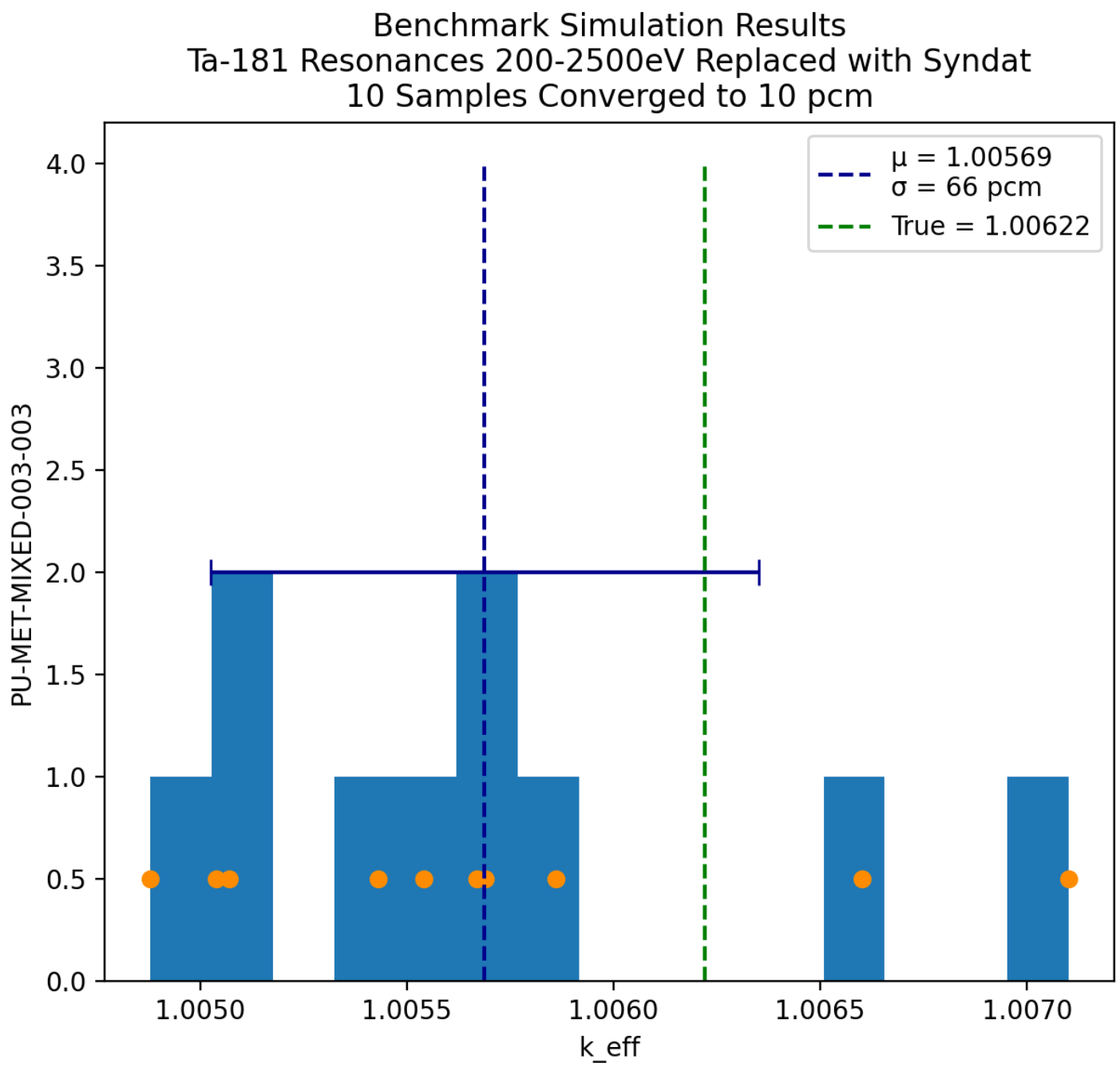
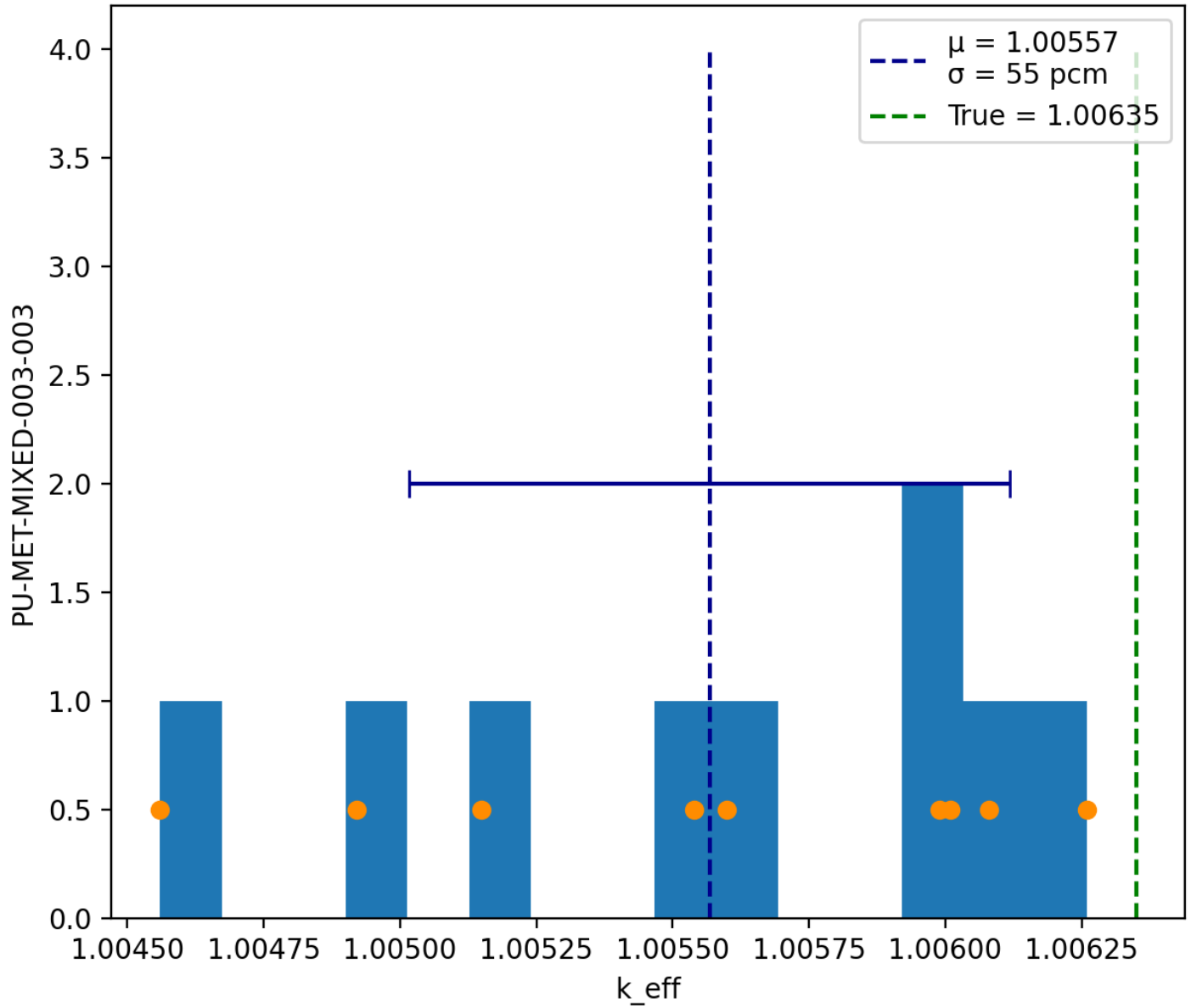





Benchmark Simulation Results
Ta-181 Resonances 200-2500eV Replaced with Syndat
18 Samples Converged to 10 pcm
μ = 1.00379
σ = 43 pcm
True = 1.00485
PU-MET-MIXED-003-003
k_eff
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1.00300
1.00325
1.00350
1.00375
1.00400
1.00425
1.00450
1.00475


Benchmark Simulation Results
Ta-181 Resonances 200-2500eV Replaced with Syndat
10 Samples Converged to 10 pcm
μ = 1.00569
σ = 66 pcm
True = 1.00622
PU-MET-MIXED-003-003
k_eff
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1.0050
1.0055
1.0060
1.0065
1.0070


Benchmark Simulation Results
Ta-181 Resonances 200-2500eV Replaced with Syndat
9 Samples Converged to 10 pcm
μ = 1.00557
σ = 55 pcm
True = 1.00635
PU-MET-MIXED-003-003
k_eff
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1.00450
1.00475
1.00500
1.00525
1.00550
1.00575
1.00600
1.00625