A Methodology for Verifiable Uncertainty Quantification

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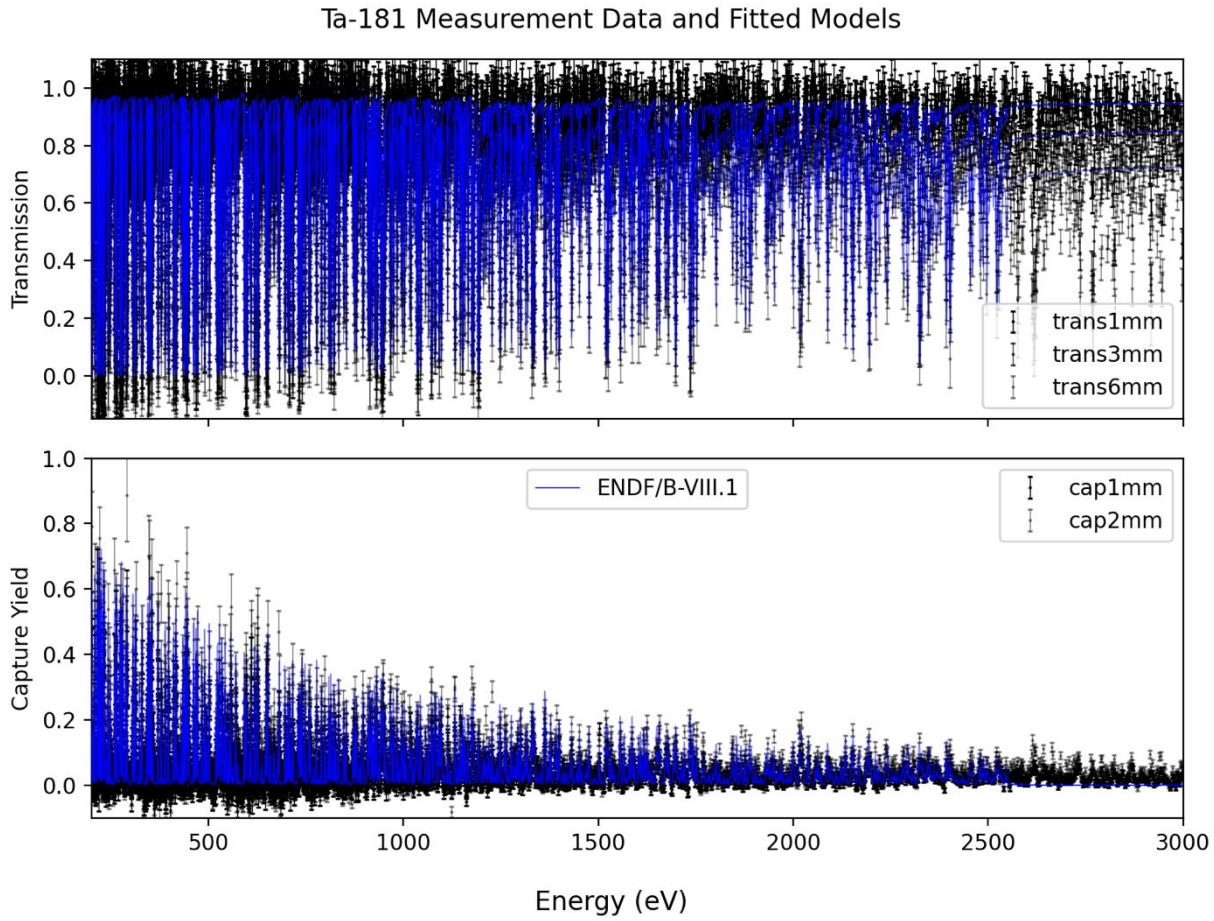
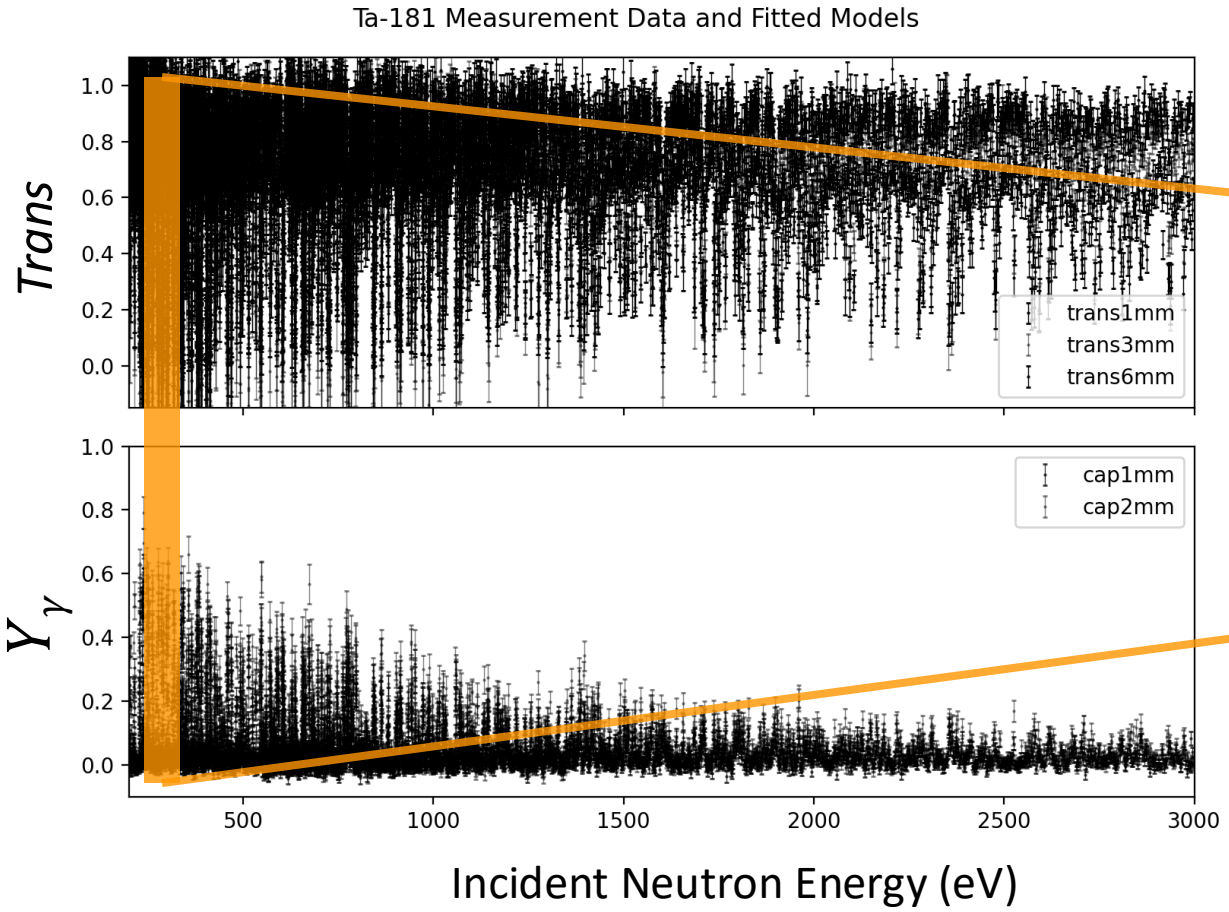
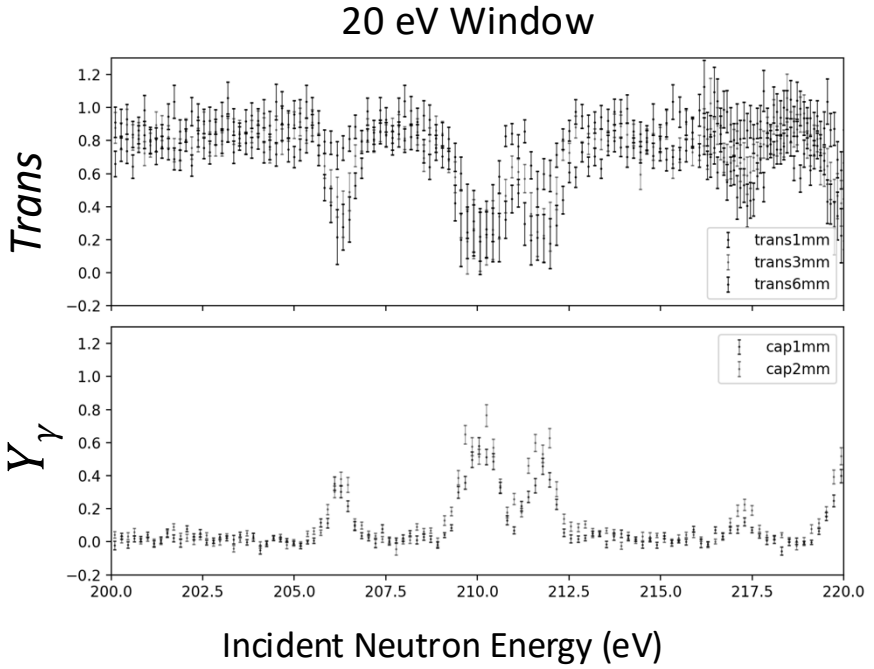
Scale of the problem

- Heavy nuclei (A>20)
- Reich Moore R-Matrix
- 100-1000 resonance parameters
  - Identify new resonances
    - Energy and partial widths (continuous)
  - Assign quantum numbers (discrete)
- 1-10 experimental data sets
- 100k-1M experimental data points



Presentation of Results





Purpose

Current uncertainty quantification (UQ) methods have known limitations:

- inaccurate when model assumptions are violated
- error corrections depend on subject matter expertise

The nuclear data community needs repeatable, accurate UQ methods. This first requires a methodology for verifying any given UQ approach.

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Current uncertainty quantification (UQ) methods have known limitations:

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The nuclear data community needs repeatable, accurate UQ methods. This first requires a methodology for verifying any given UQ approach.

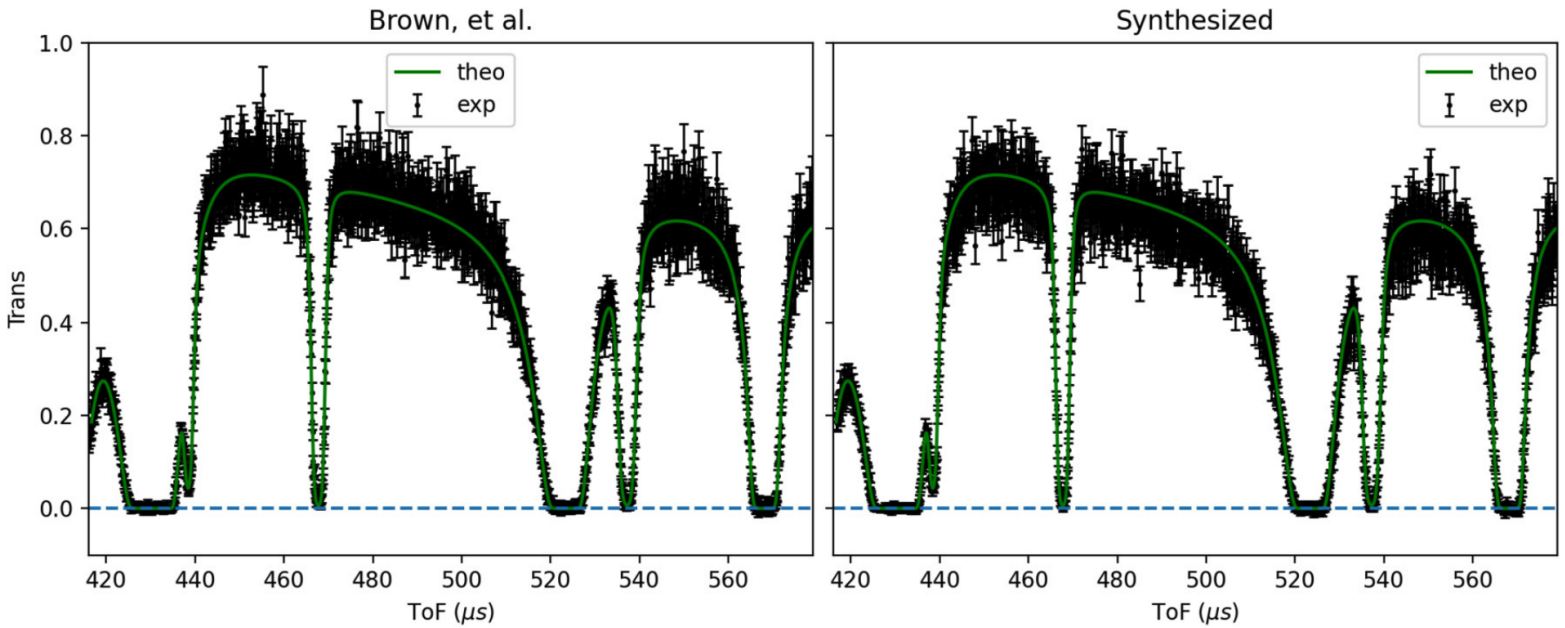
We propose a methodology which leverages high-fidelity synthetic data for verifying any candidate UQ approach.

Syndat: Reproducible Synthetic Data

Walton, Brown, Fritsch, *et al.* [1] provide

> *"a generative model for the experimental observables produced by a determined total cross section in a neutron time-of-flight (TOF) transmission experiment,"*

and accompanying open source code [2].



[1] N. Walton, J. Brown, W. Fritsch, D. Brown, G. Nobre, and V. Sobes, "Methodology for physics-informed generation of synthetic neutron time-of-flight measurement data," *Computer Physics Communications*, vol. 294, p. 108 927, 2024.

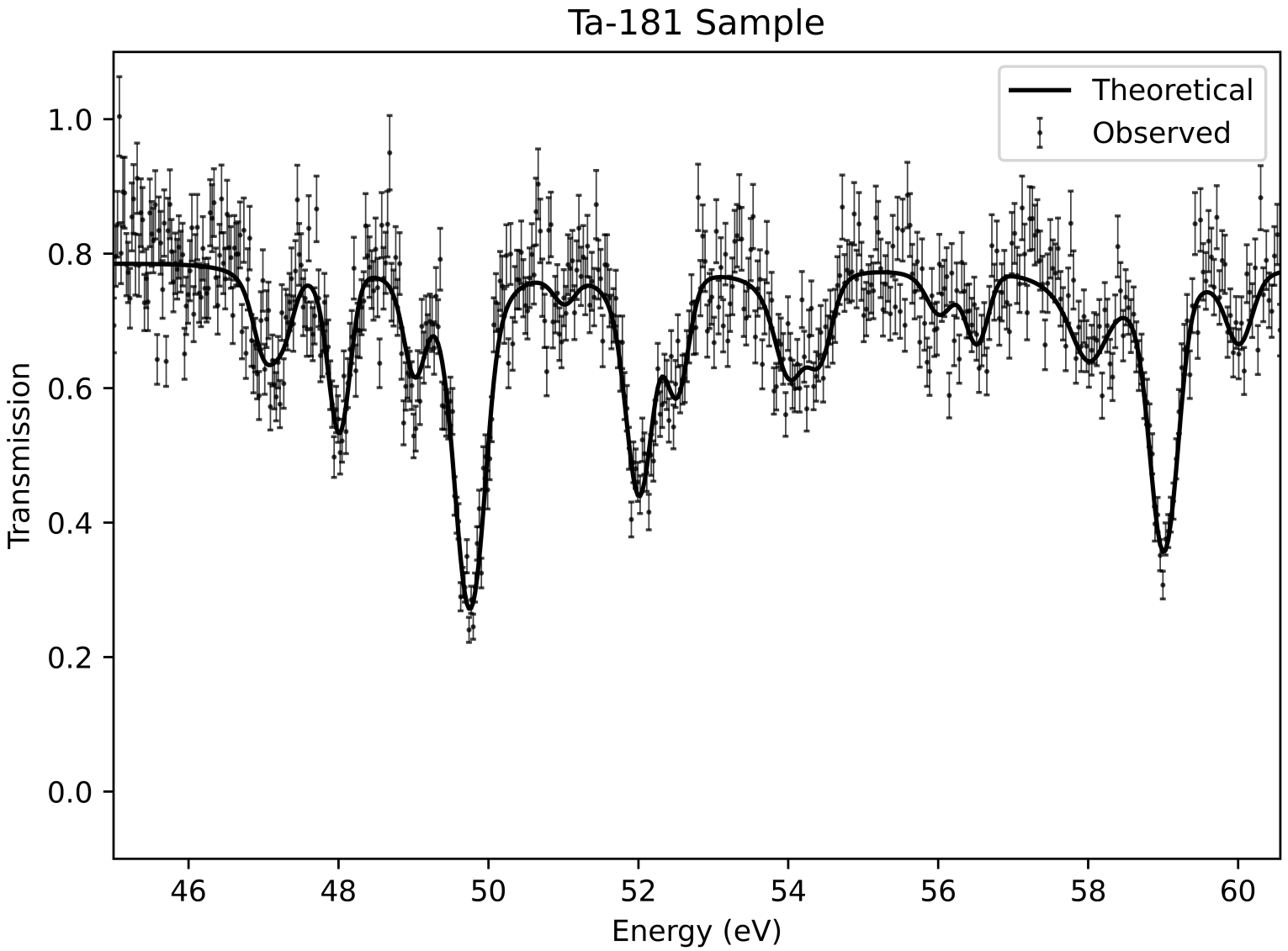
SAMMY UQ Limitations

Updated Users' Guide to SAMMY, Section IV.E.6:

> *"The posterior resonance parameter covariance matrix (RPCM) produced by SAMMY is a accurate representation of the uncertainties in the R-matrix evaluation. Nevertheless, uncertainties for evaluated cross sections reproduced by propagating the RPCM have historically been regarded as 'too small.'" [3]*

[3] N. M. Larson, "Updated users' guide for sammy: Multilevel r-matrix fits to neutron data using bayes' equations," ORNL, ORNL, Oak Ridge, TN, Tech. Rep. ORNL/TM-9179/R8, 2008, Section IV.E.6.

Ta-181 Example



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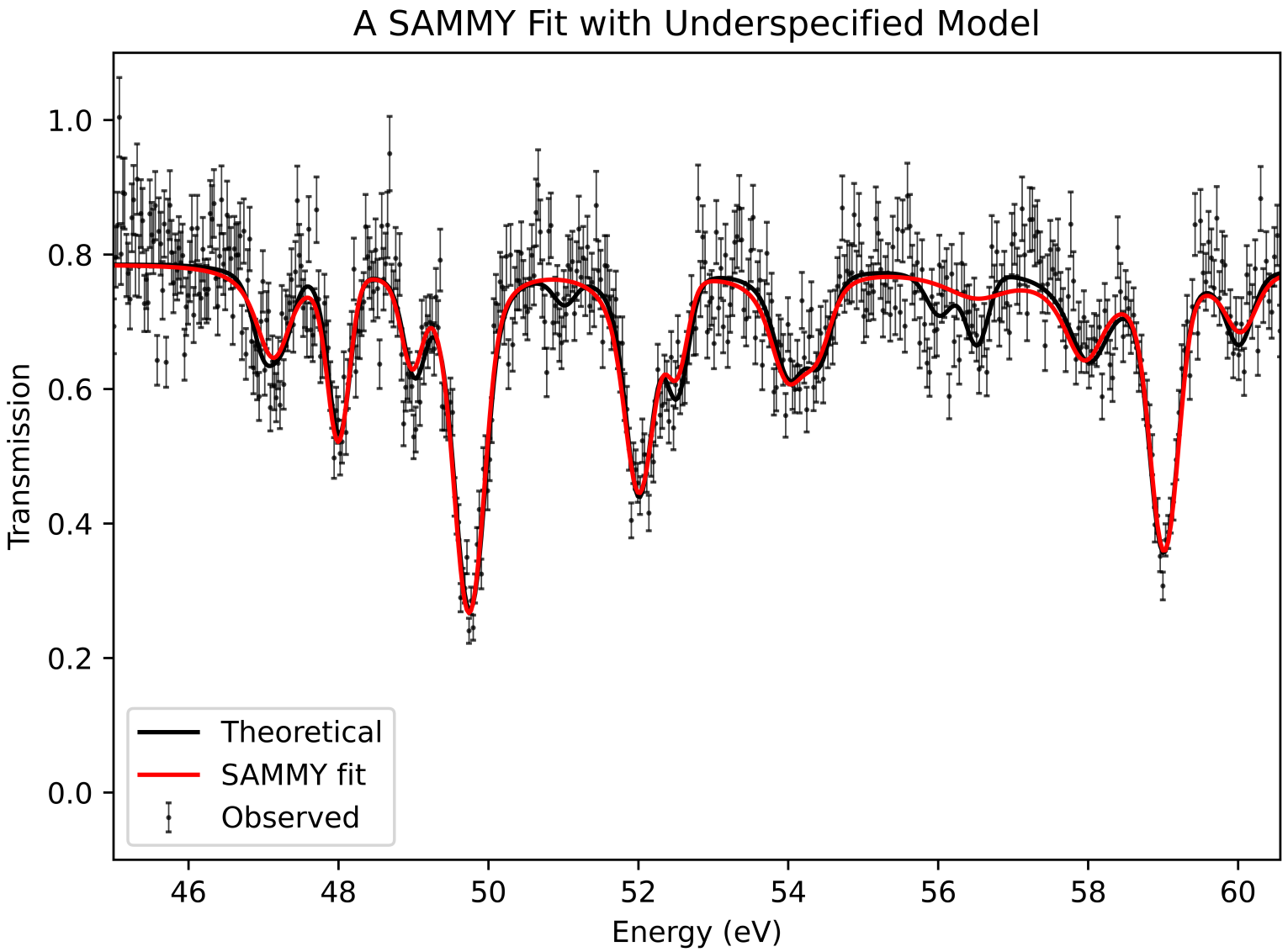

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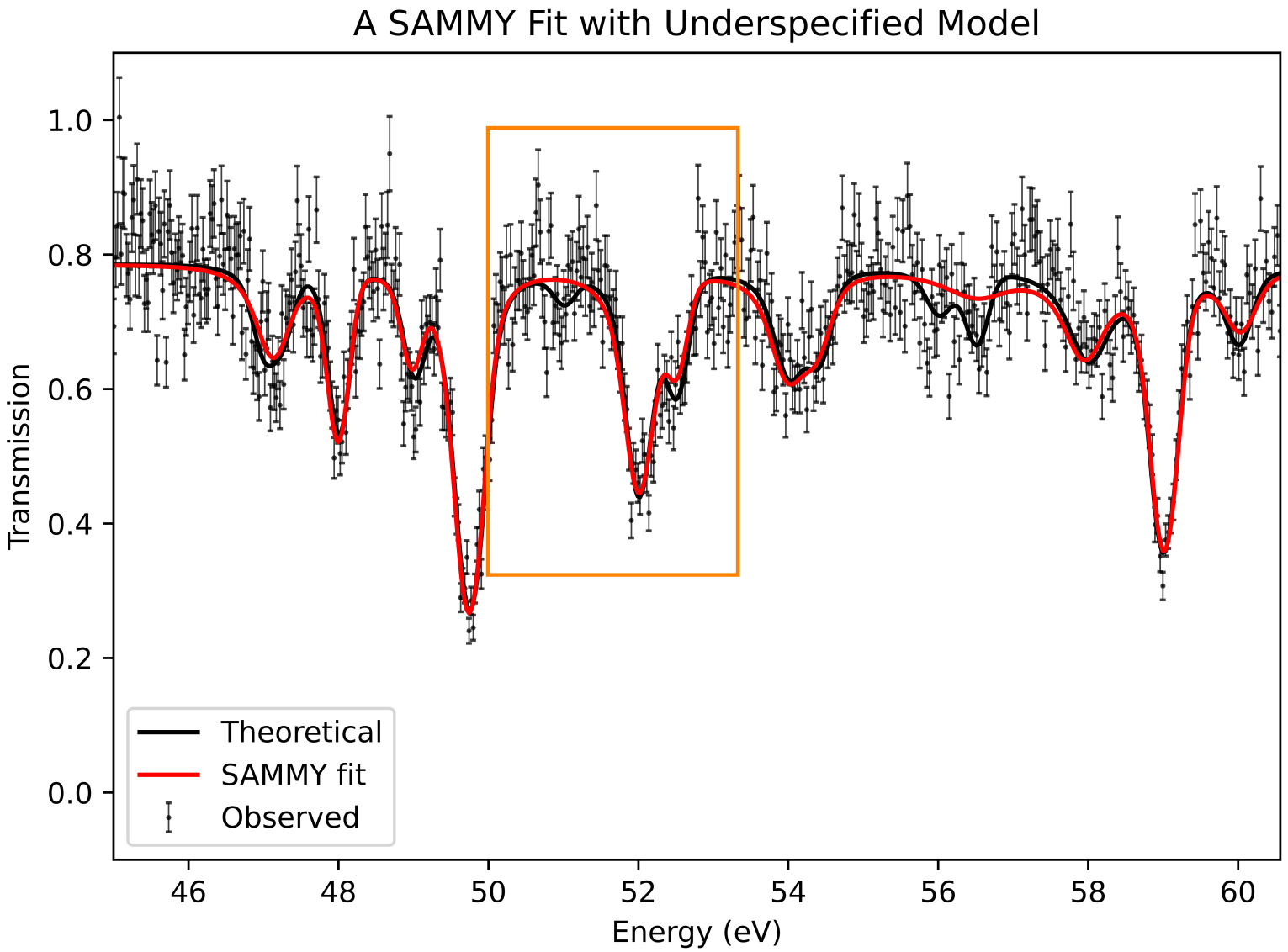

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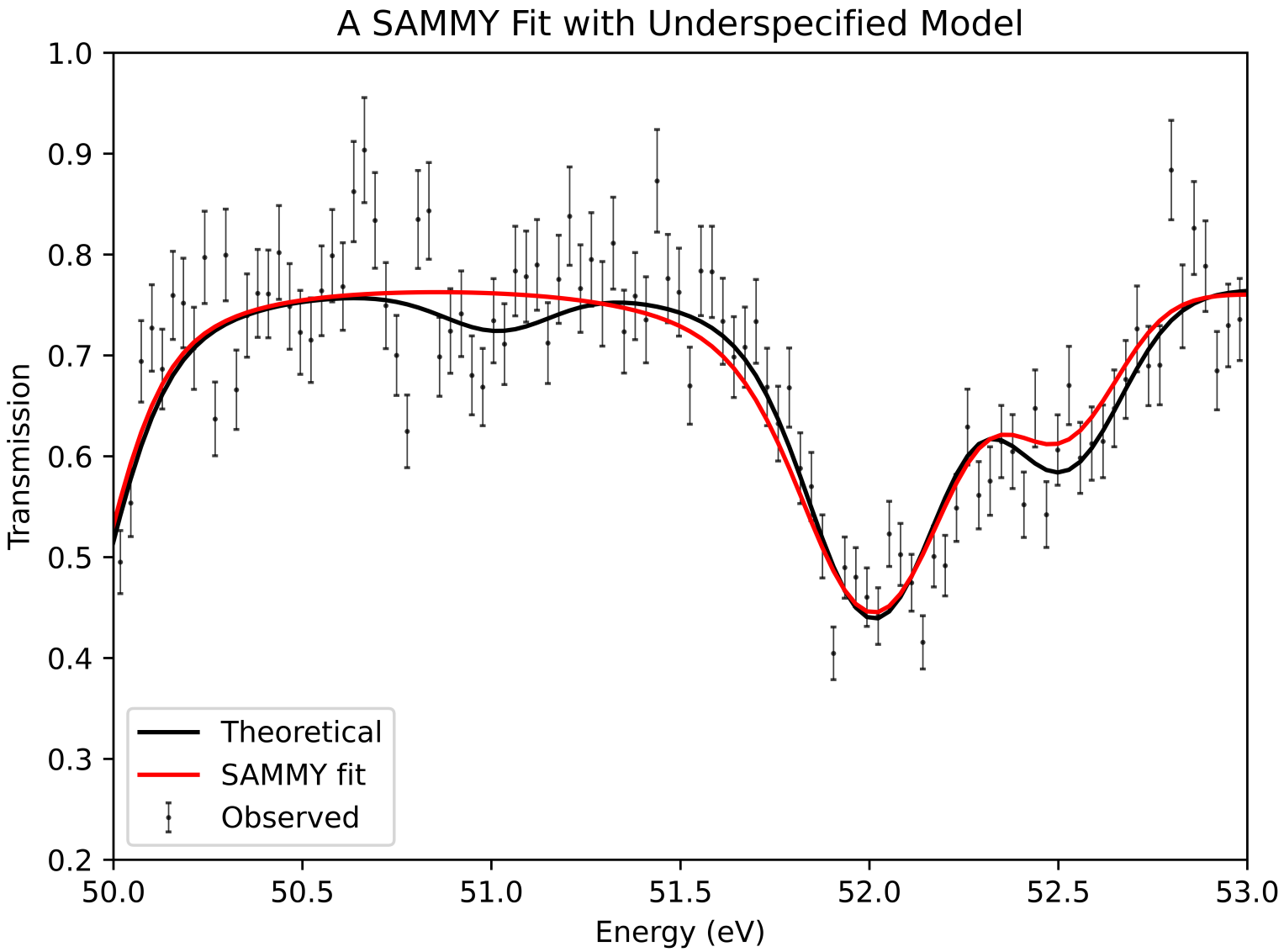

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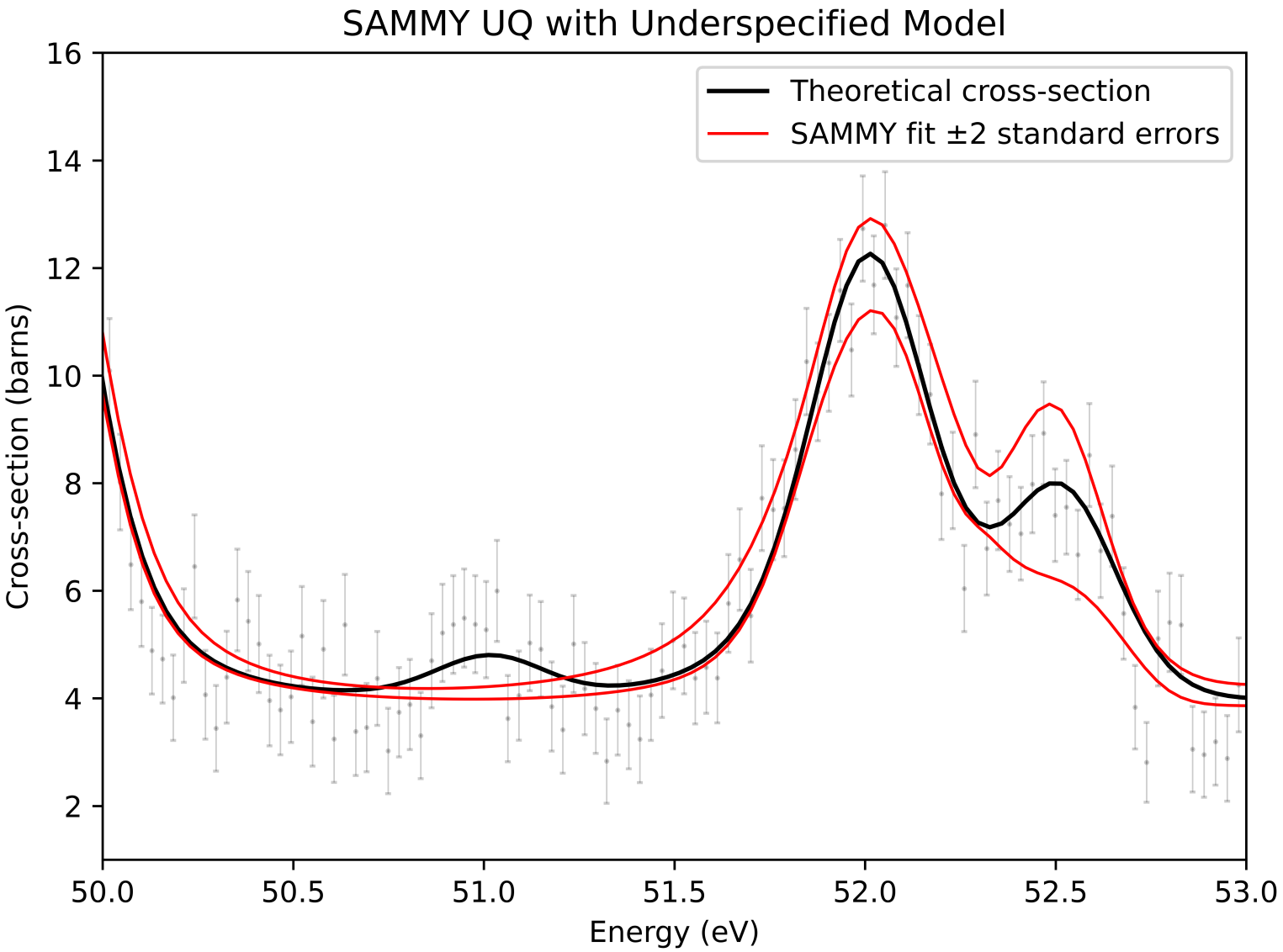

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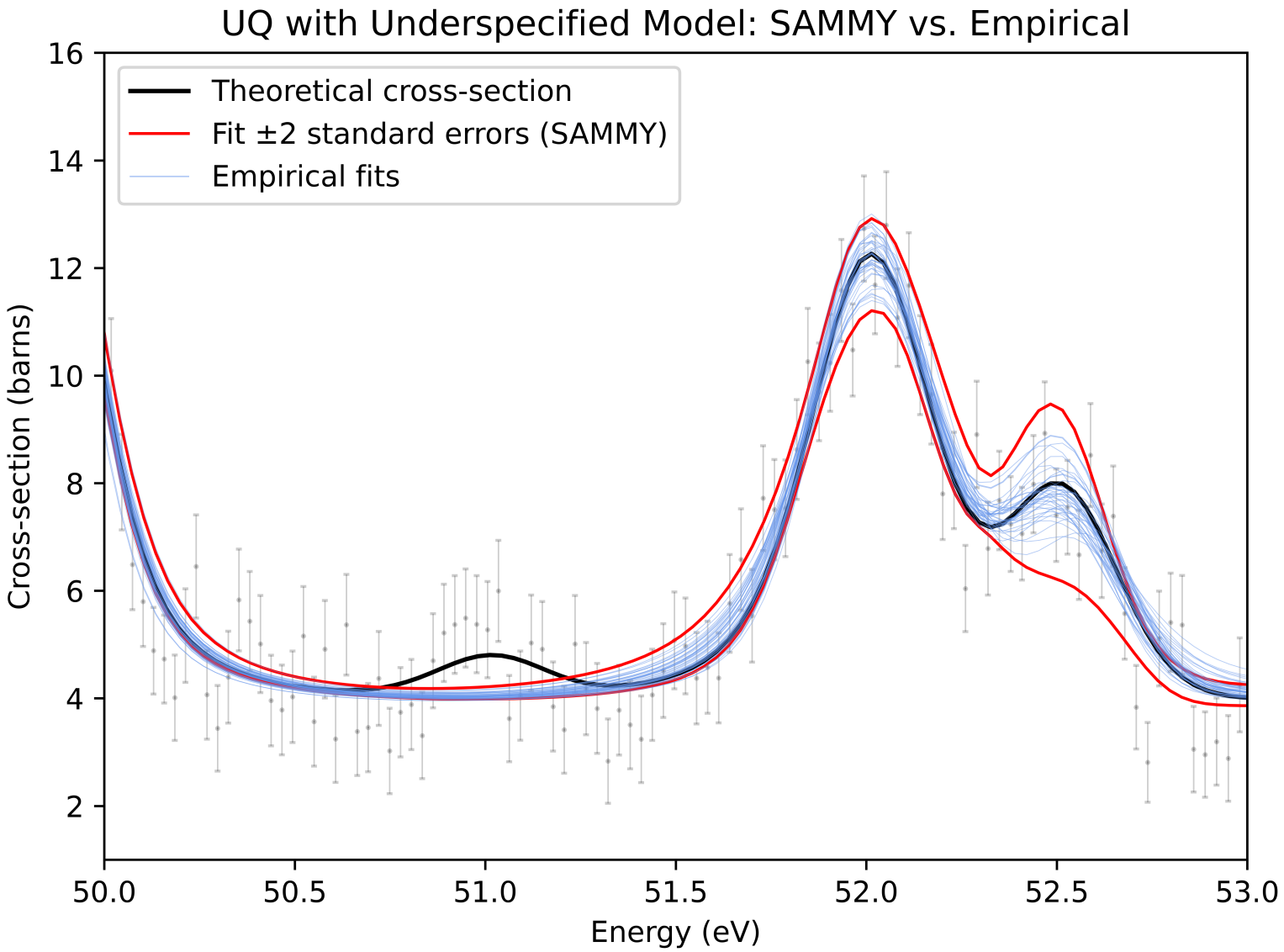

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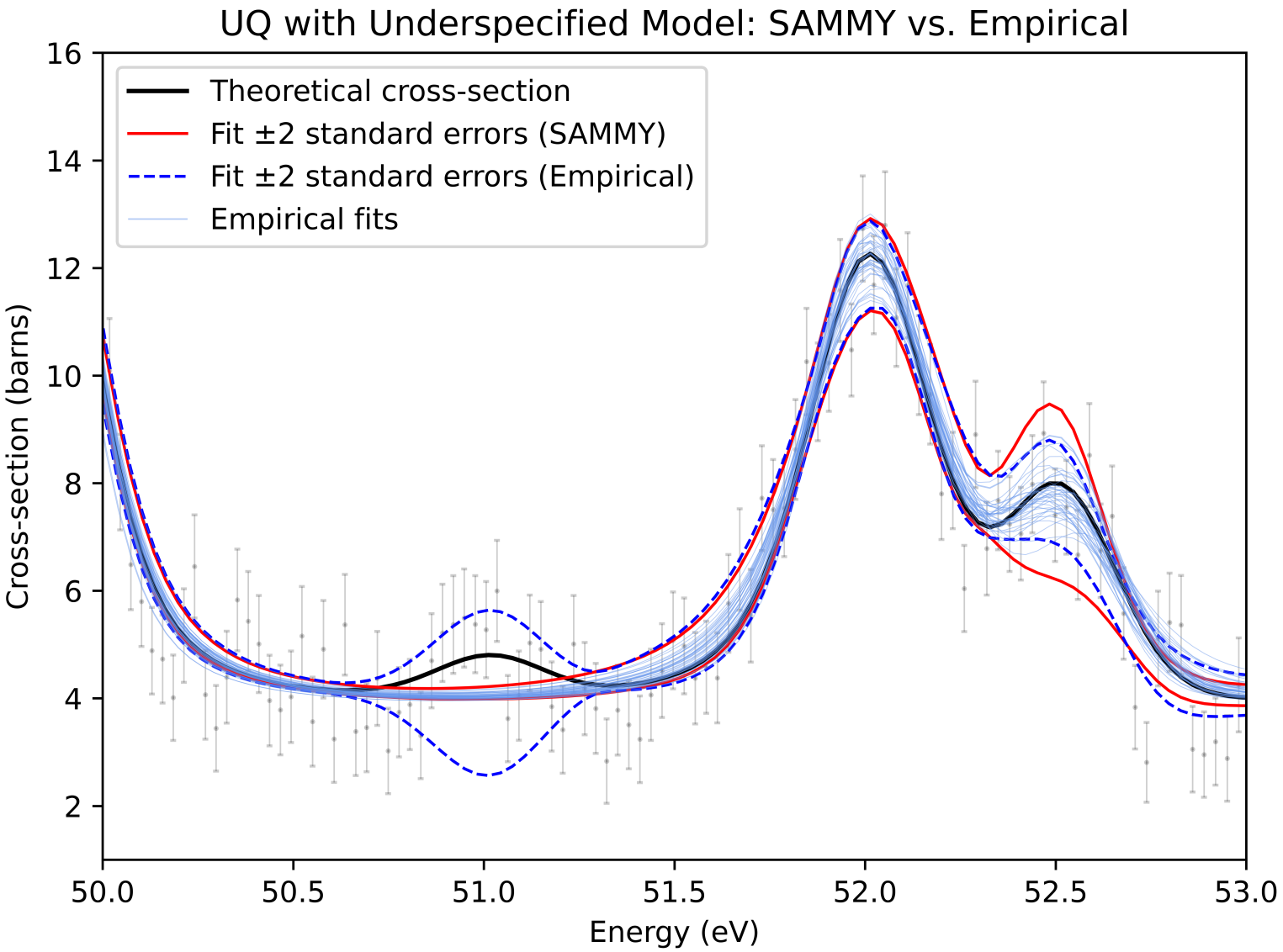

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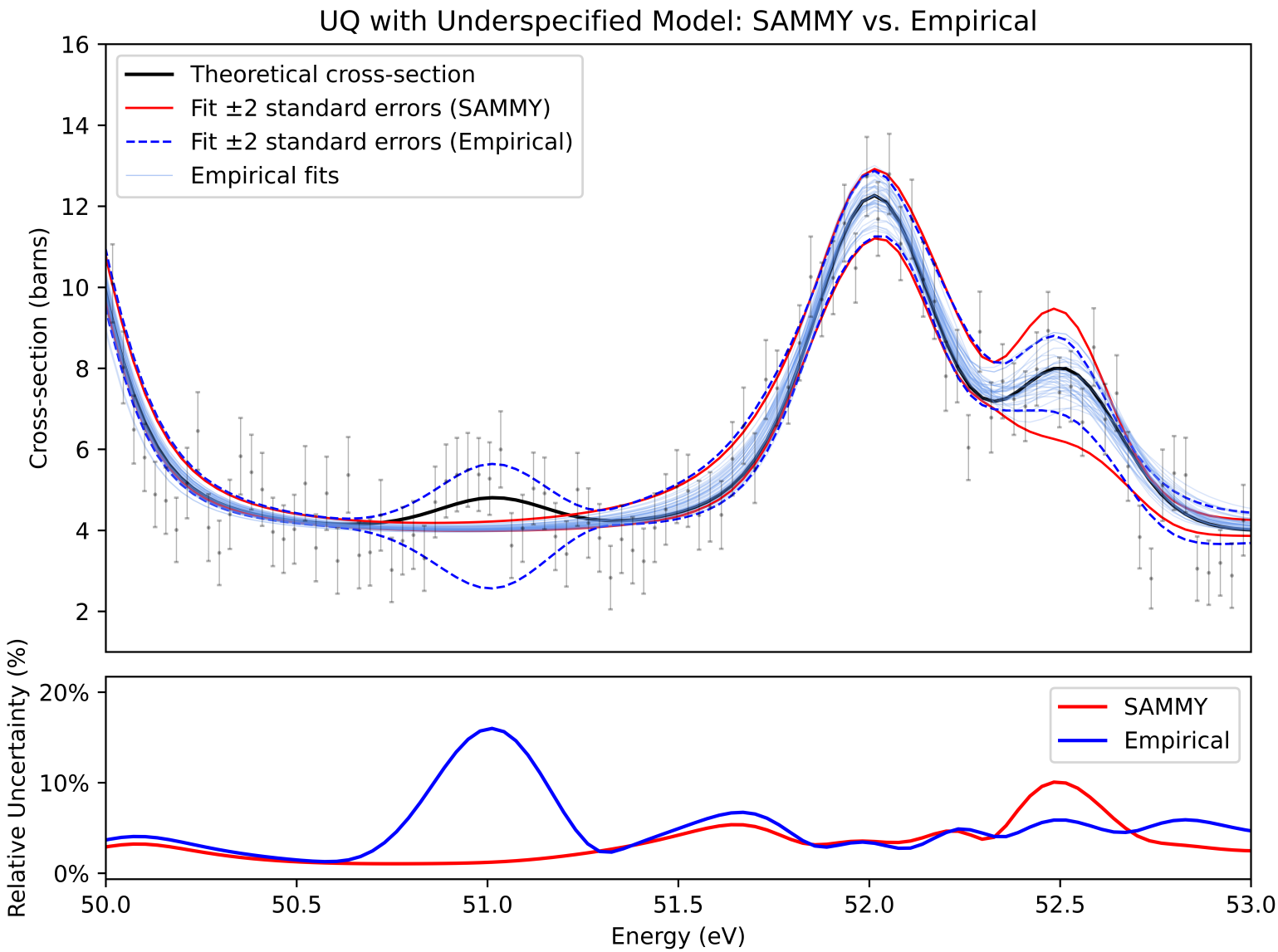

Pause and reflect

What have we shown?

- Use synthetic data to quantify the impact of model assumption violations on UQ accuracy.

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What's next?

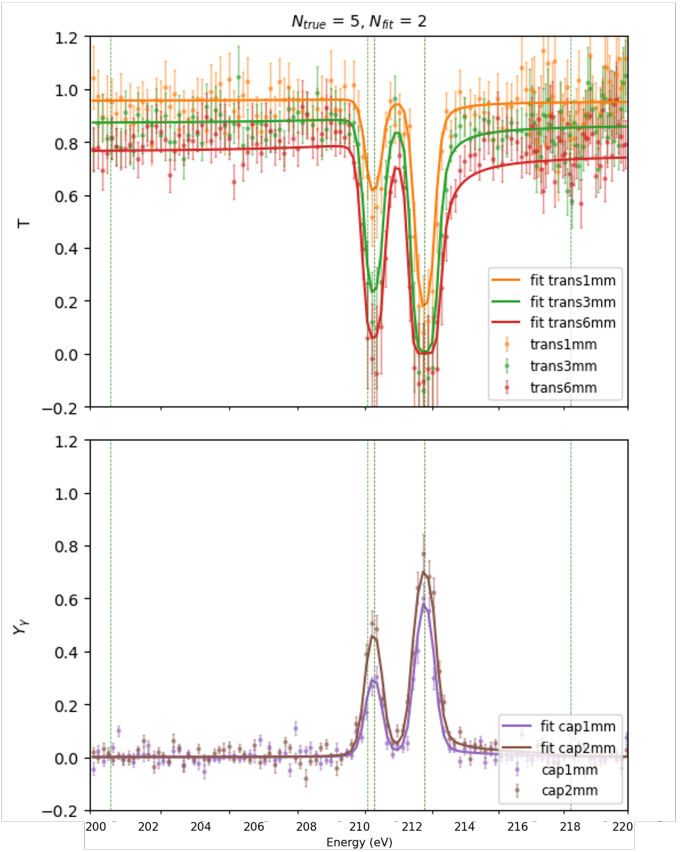
- Use synthetic data to develop a repeatable methodology for generating verifiably accurate UQ.

Automated Fitting

An overview of AutoFit:

- Dense feature bank of many resonances
- Iteratively step down model cardinality and fit
- Use cross-validation to determine optimal cardinality

Valuable information for UQ is contained in higher-cardinality model fits.



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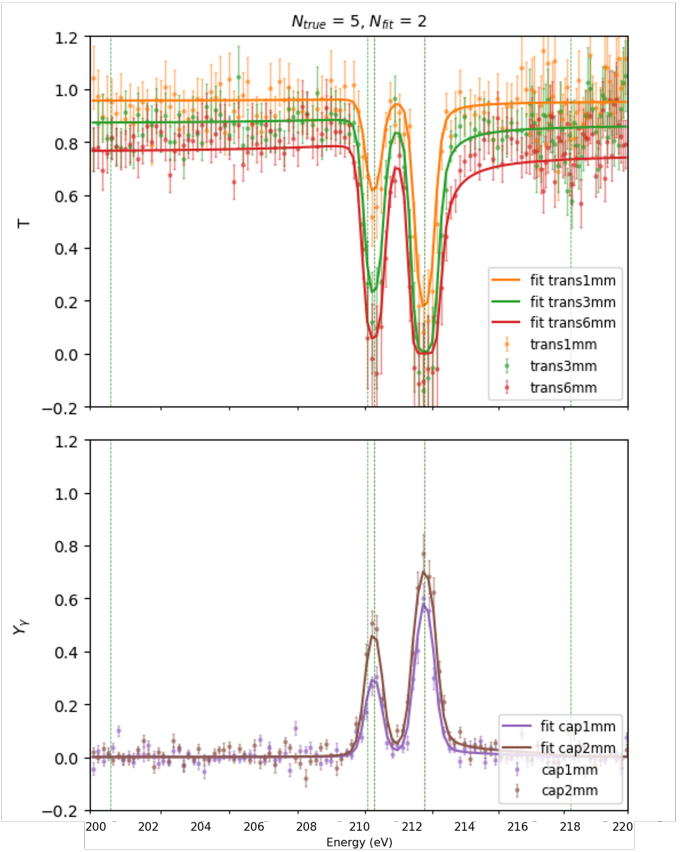
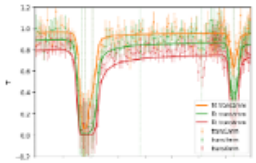


Key idea: SAMMY cross section covariance matrices computed at multiple cardinalities for a given sample can be used as features for machine learning parameters which can be applied to new data for improved UQ.

Process

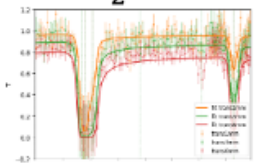
Training Data

$k_1 = 2$



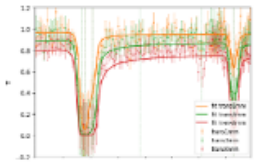
$\rightarrow C_1$

$k_2 = 3$



$\rightarrow C_2$

$k_{10} = 11$



$\rightarrow C_{10}$

Learn parameters that map SAMMY covariances to empirical.

$$\hat{\beta}_{1:10} = \underset{\beta_{0:10}}{\operatorname{argmin}}(\|E - (\beta_0 + \beta_1 C_1 + \cdots + \beta_{10} C_{10})\|_2)$$

Process

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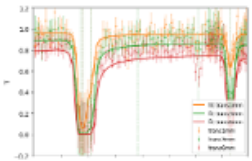

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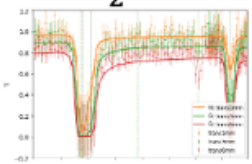

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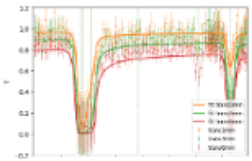

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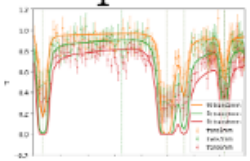
$C_M = \_ + \_C_1 + \cdots + \_C_{10}$

We want to improve the UQ accuracy by using information contained in SAMMY covariances for the test data.

Test Data

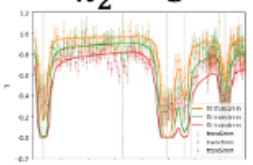
$k_1 = 4$

$C_1 \leftarrow$



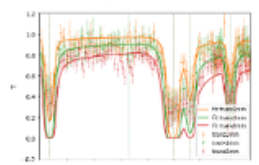
$k_2 = 5$

$C_2 \leftarrow$



$k_{10} = 13$

$C_{10} \leftarrow$



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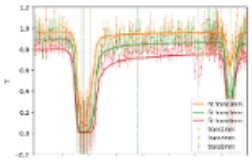

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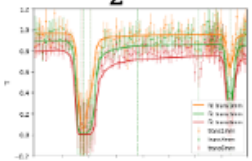

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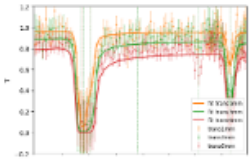

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$$C_M = \hat{\beta}_0 + \hat{\beta}_1 C_1 + \cdots + \hat{\beta}_{10} C_{10}$$

Apply learned parameters on user data to obtain improved UQ.

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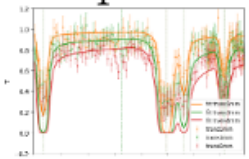
$C_1 \leftarrow$ 

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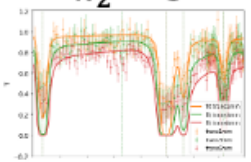
$C_2 \leftarrow$ 

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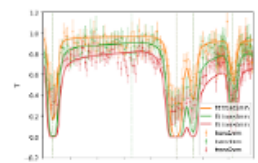
$C_{10} \leftarrow$ 

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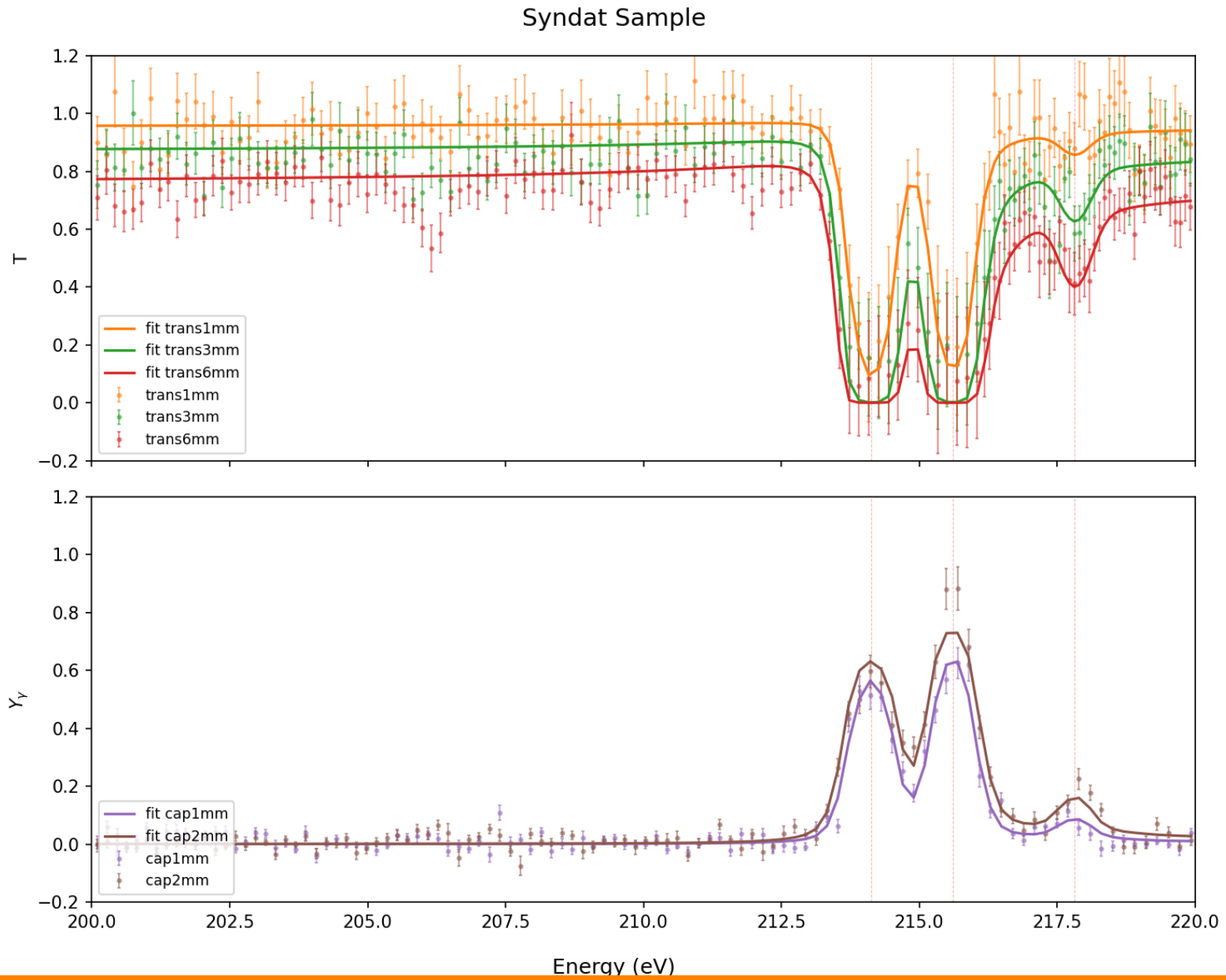

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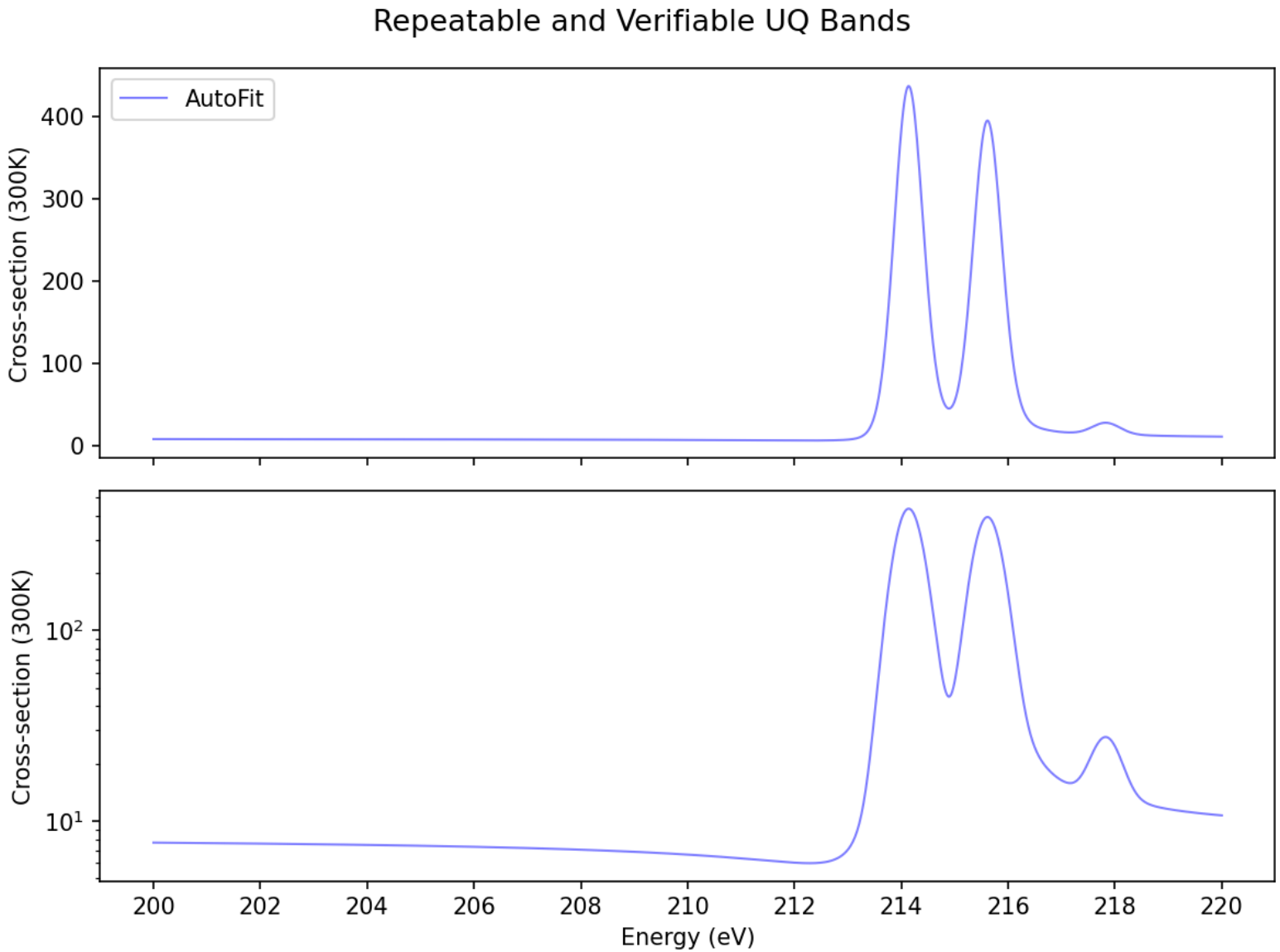

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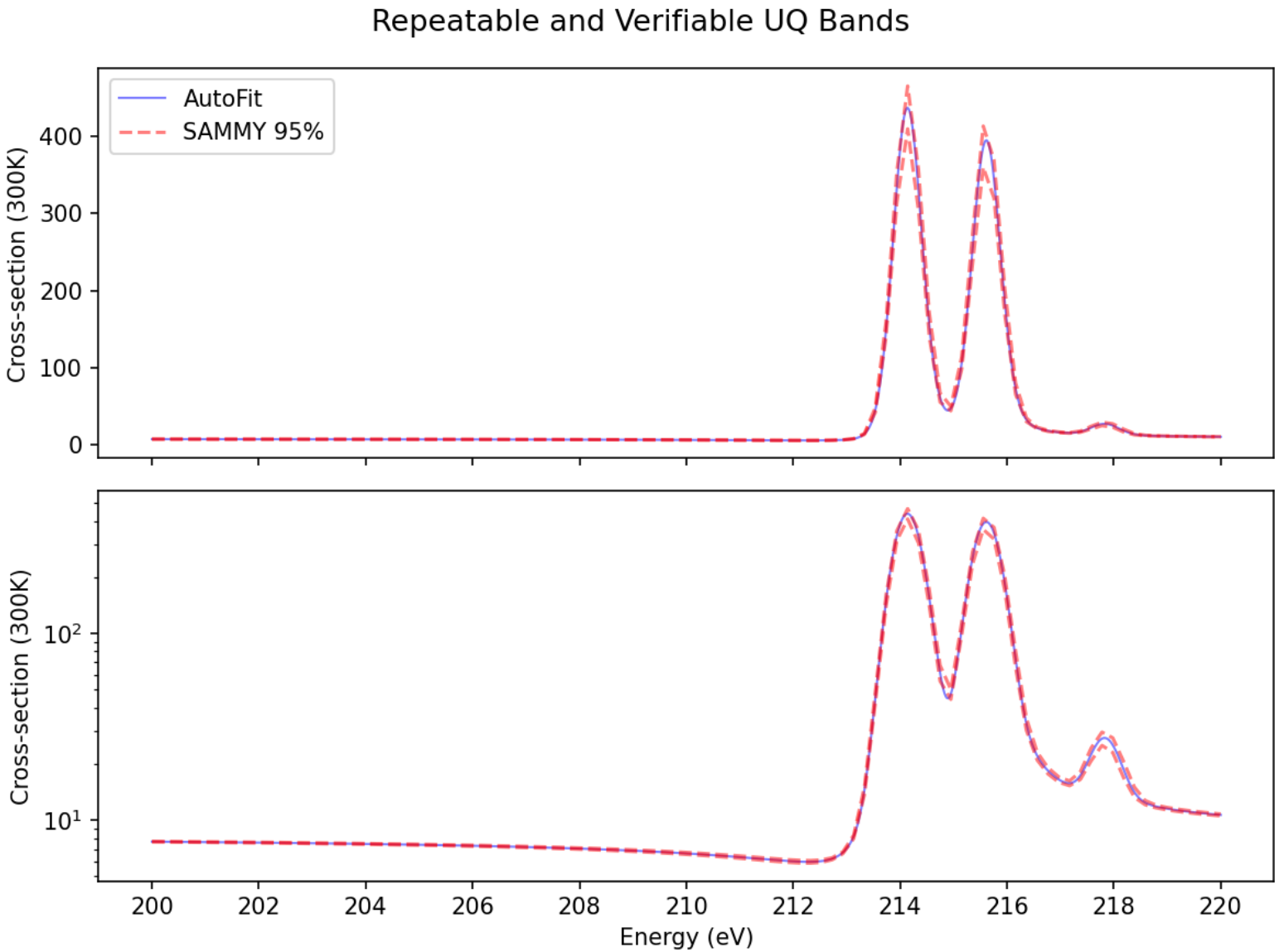

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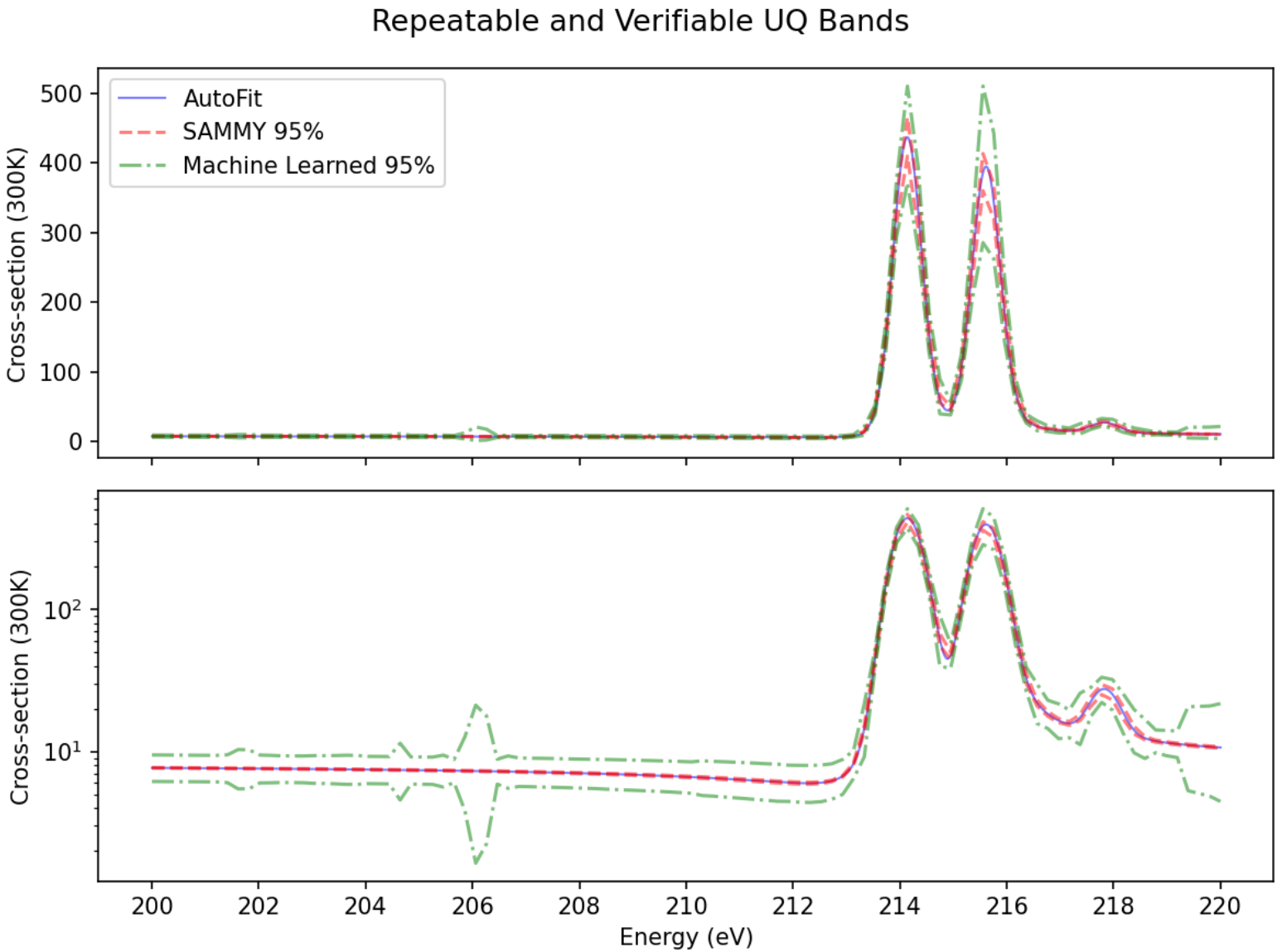

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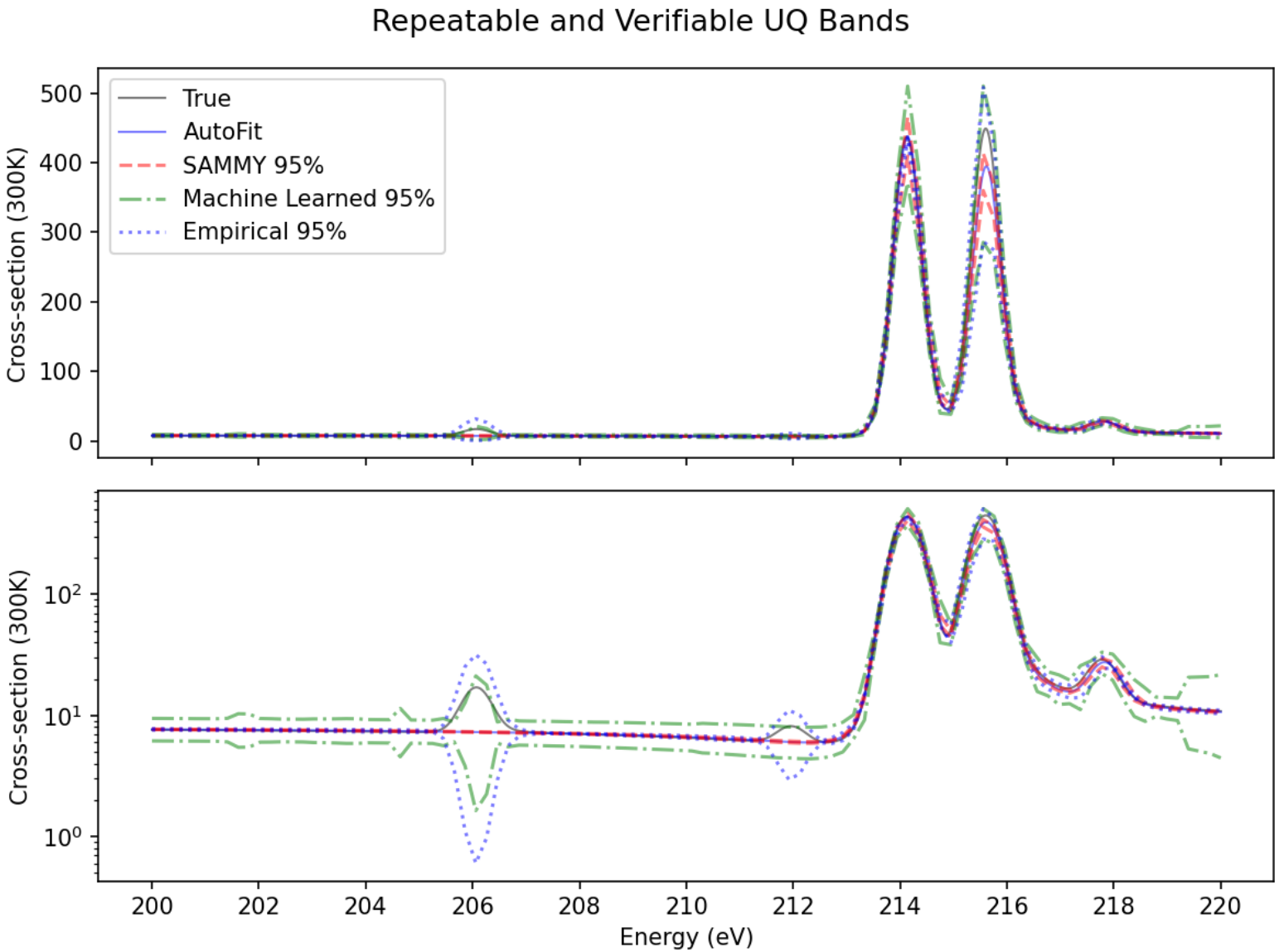

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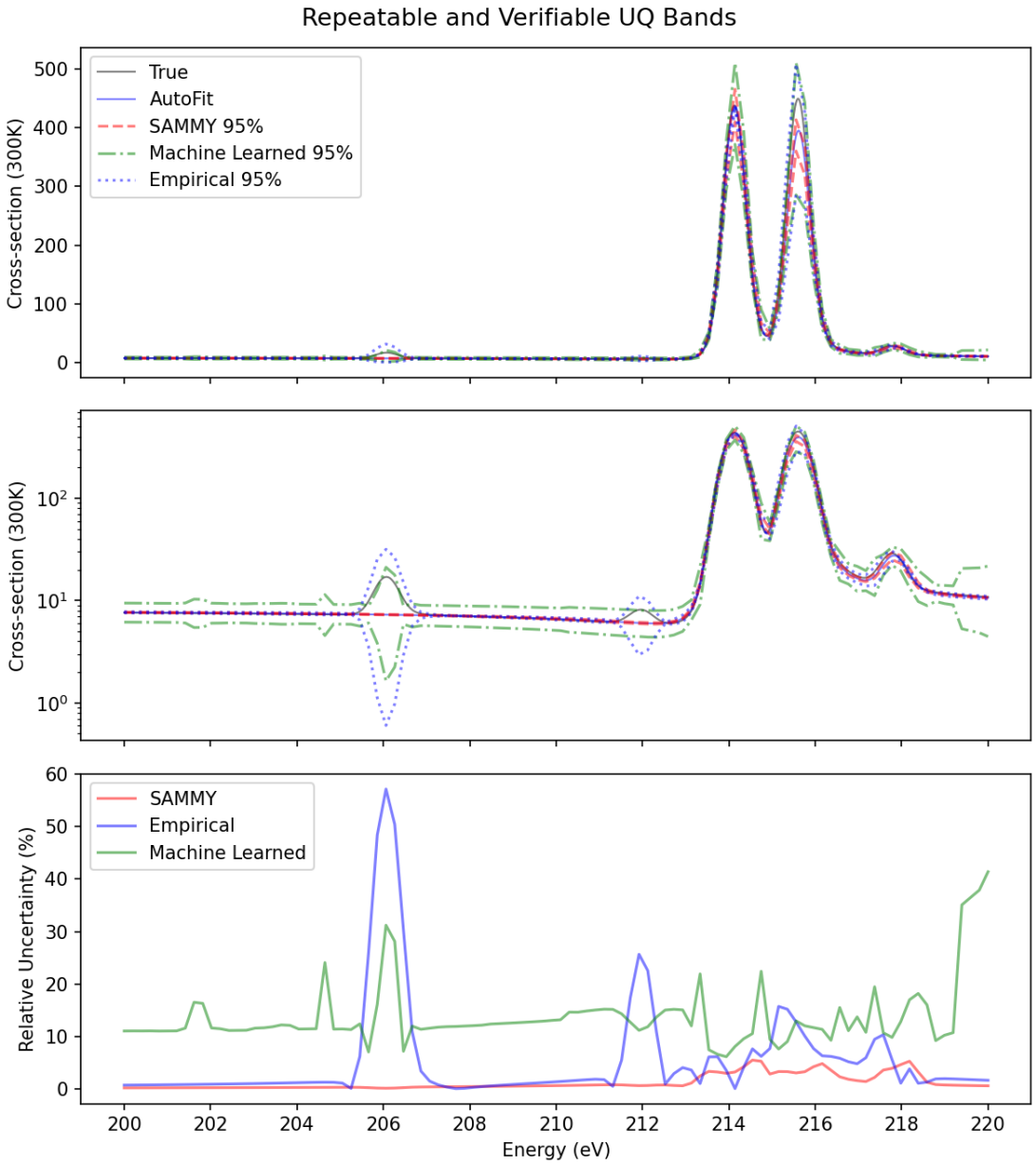
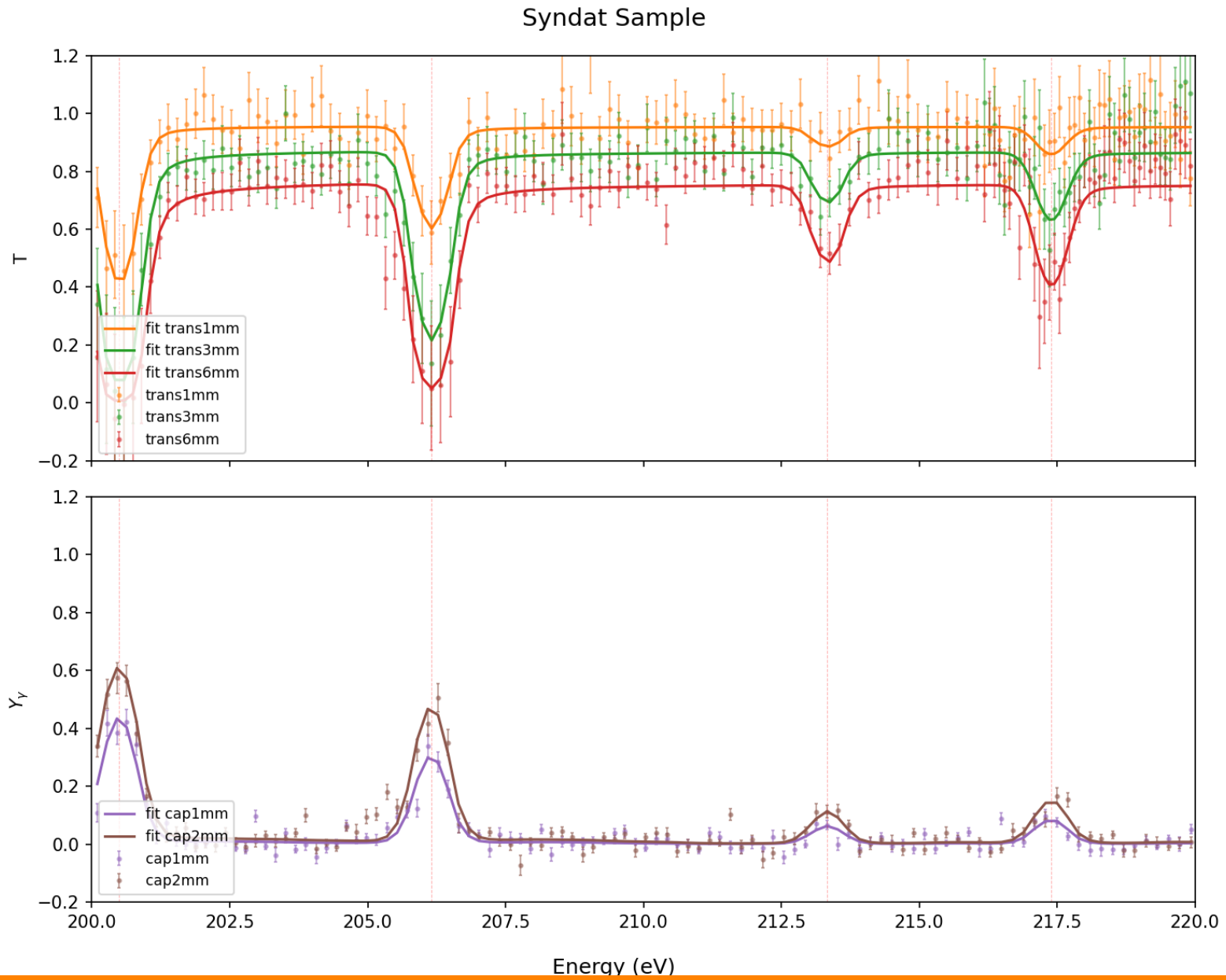


Example 2



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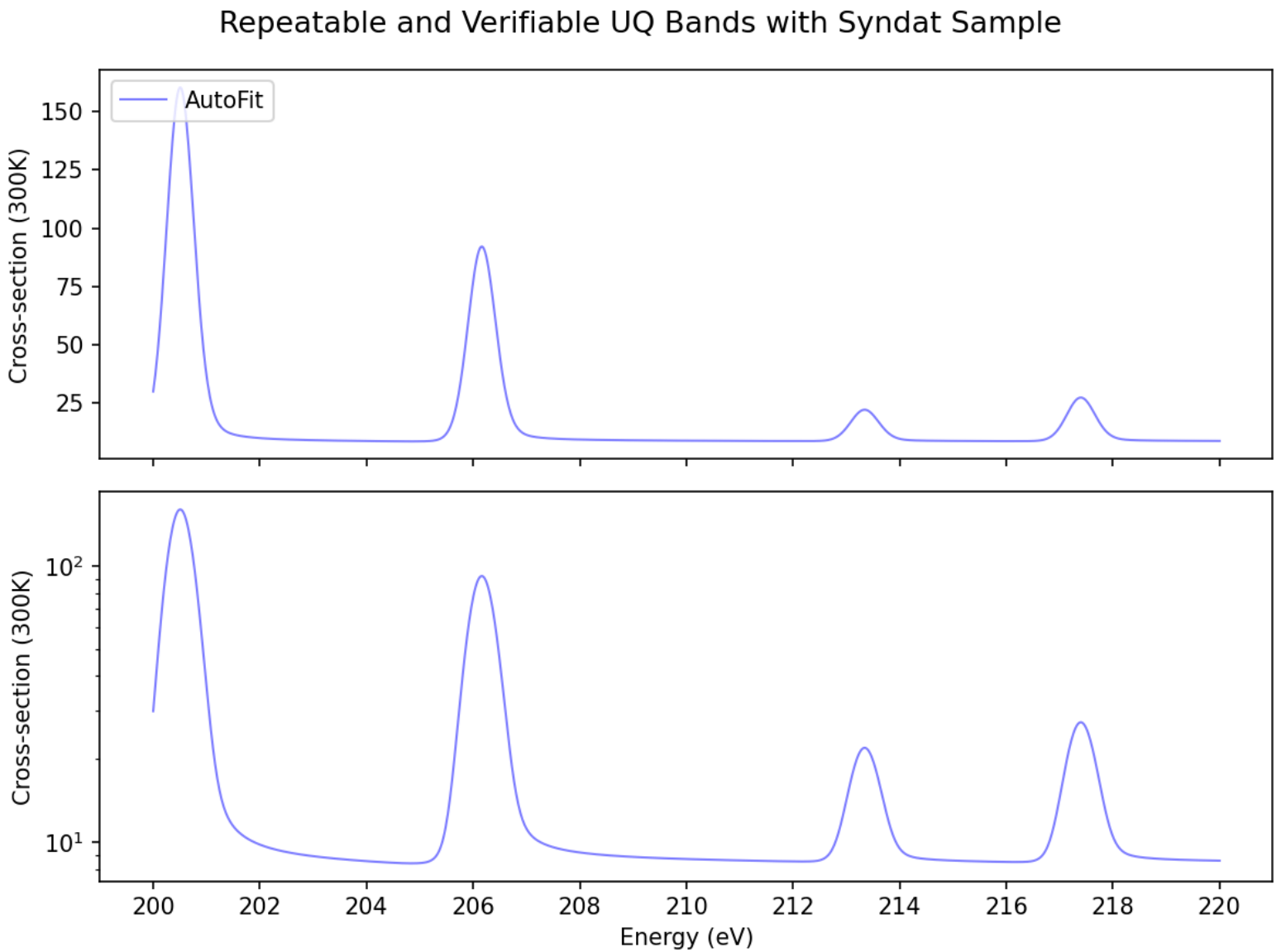

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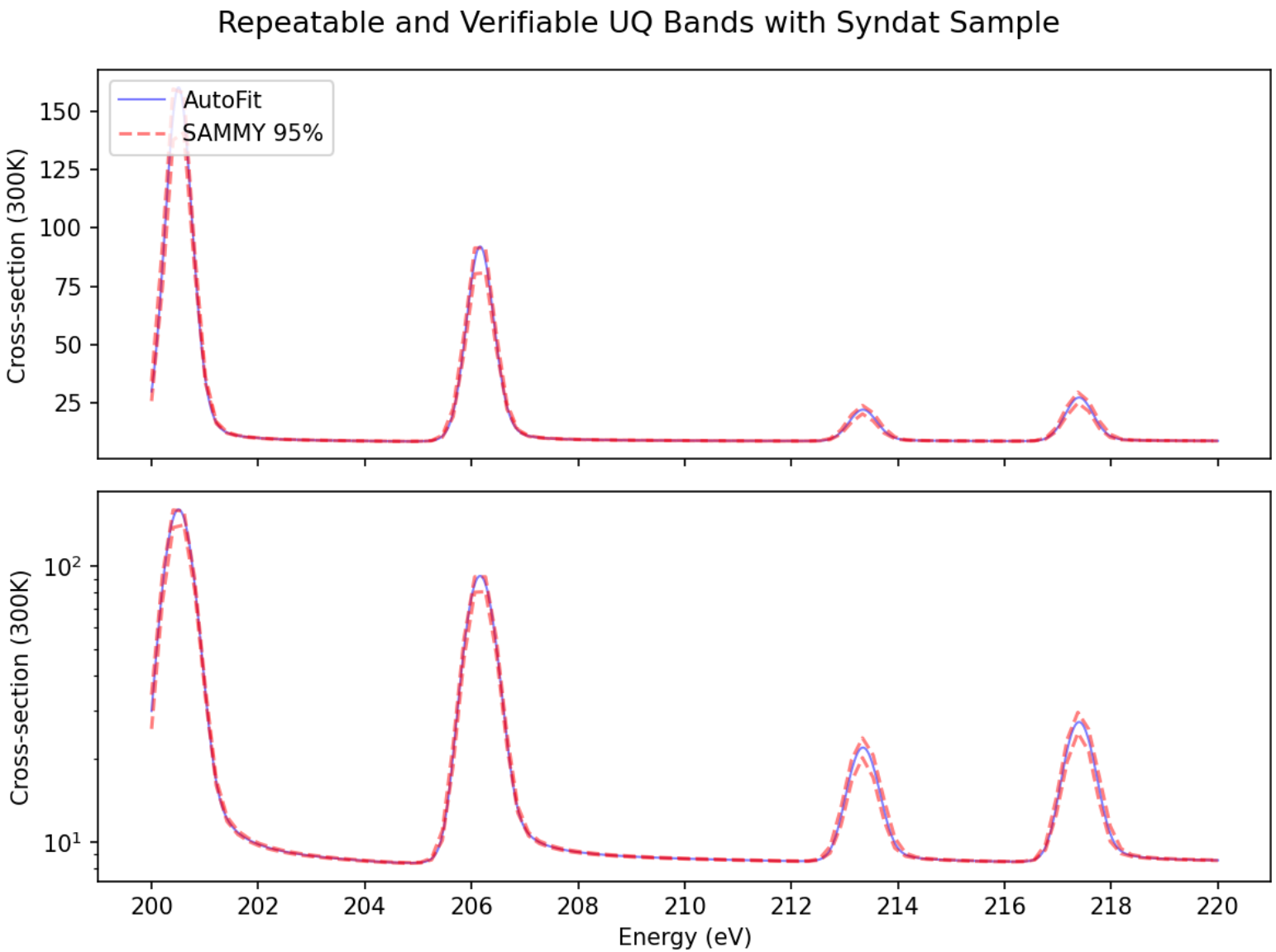

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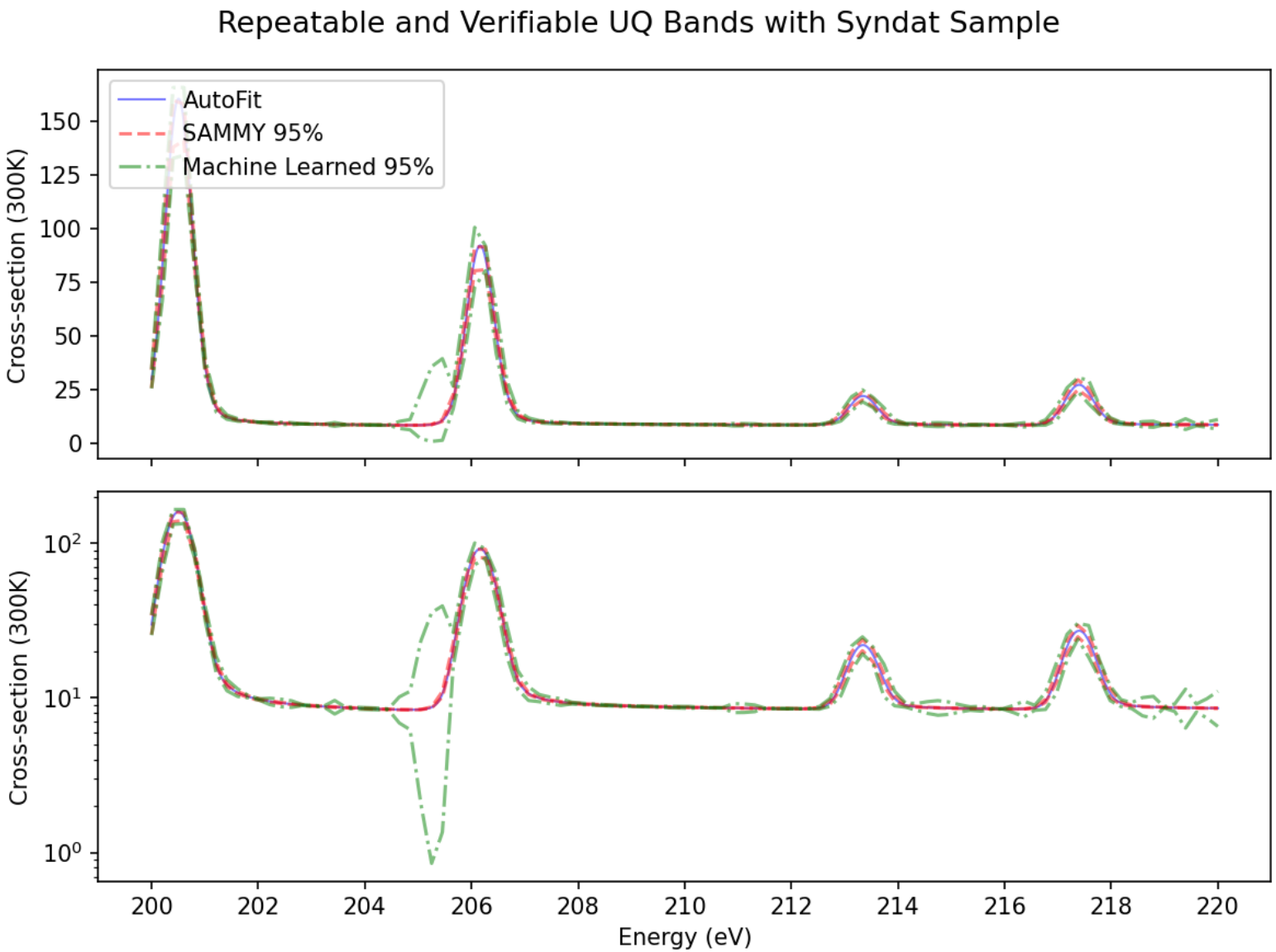

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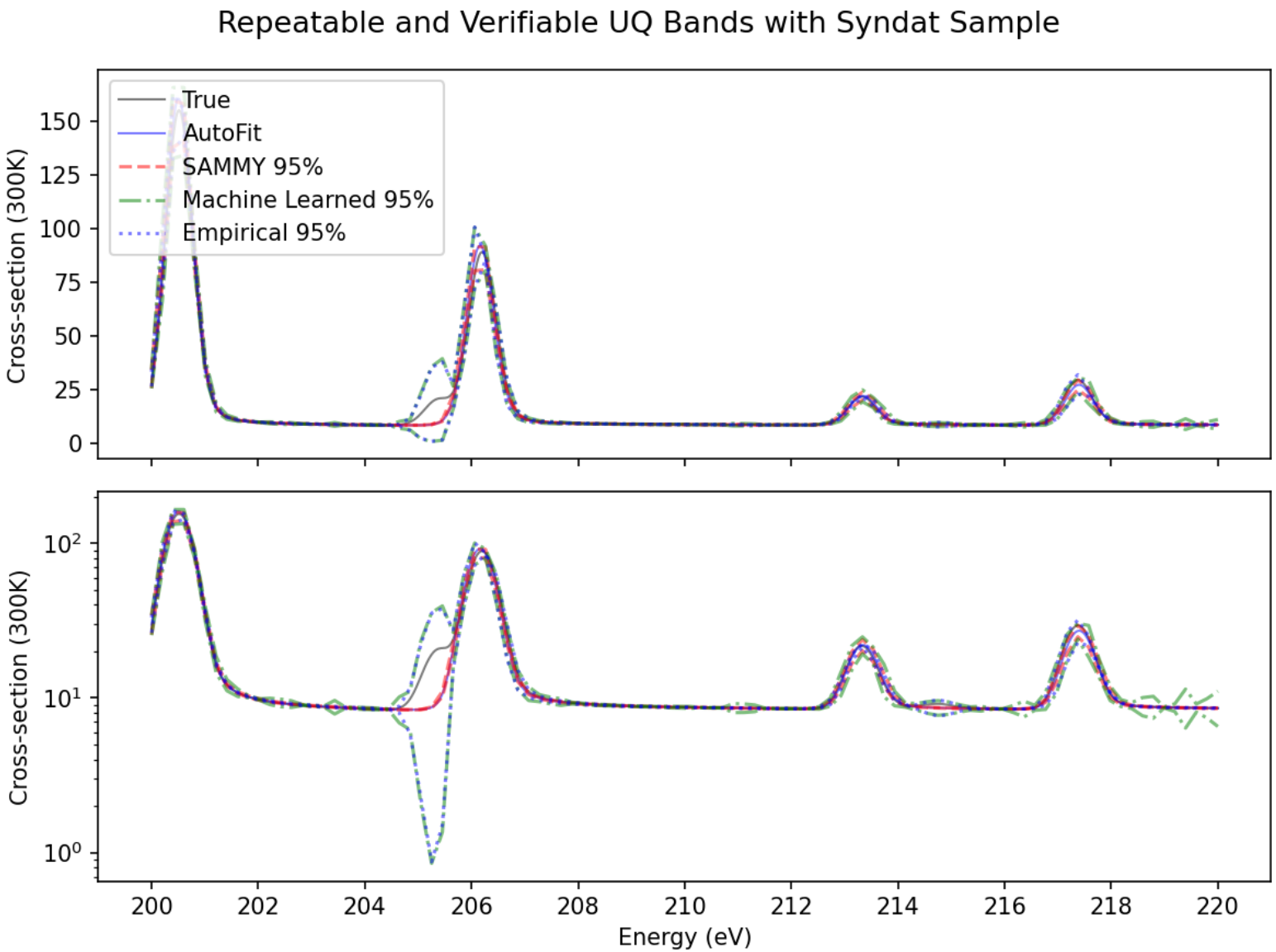

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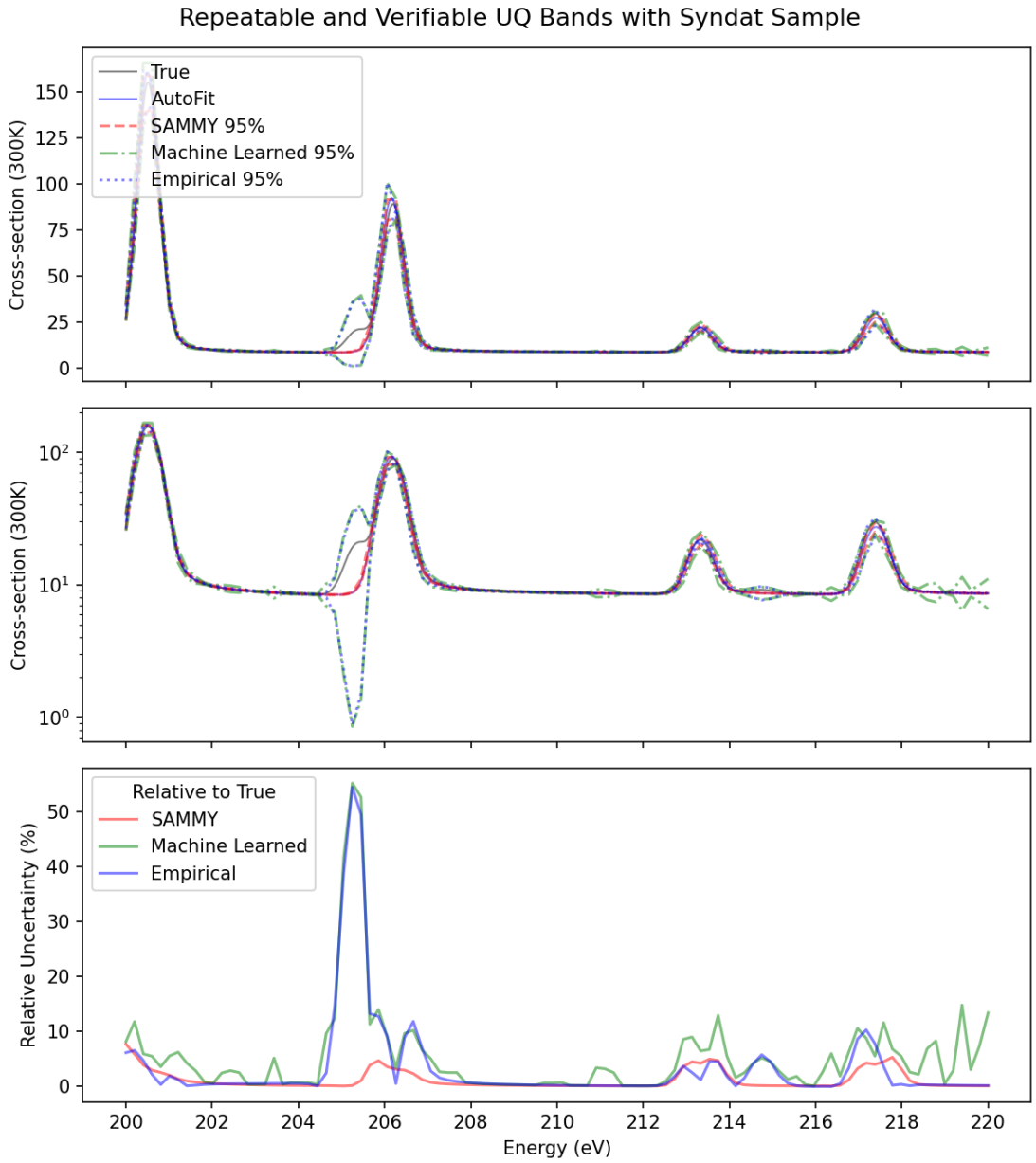
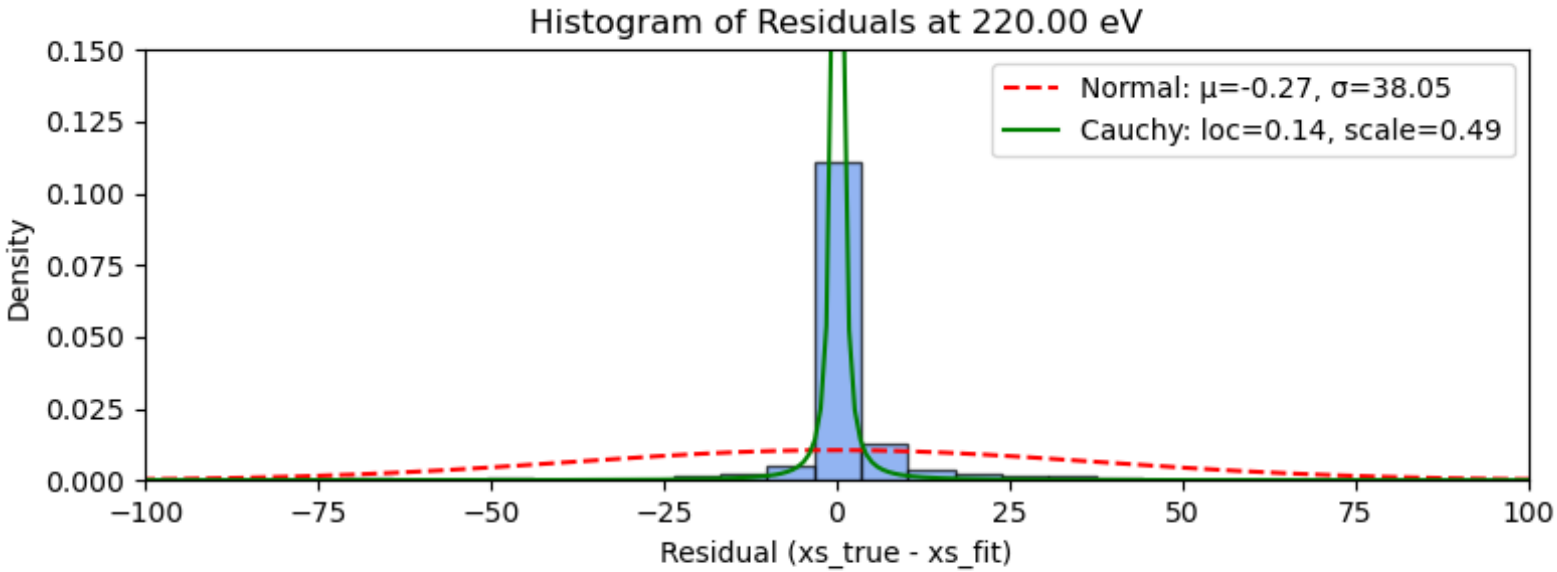
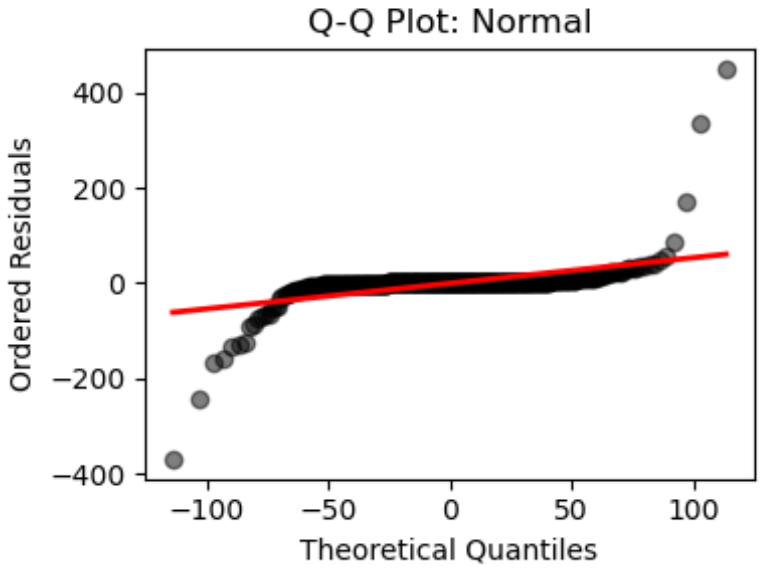
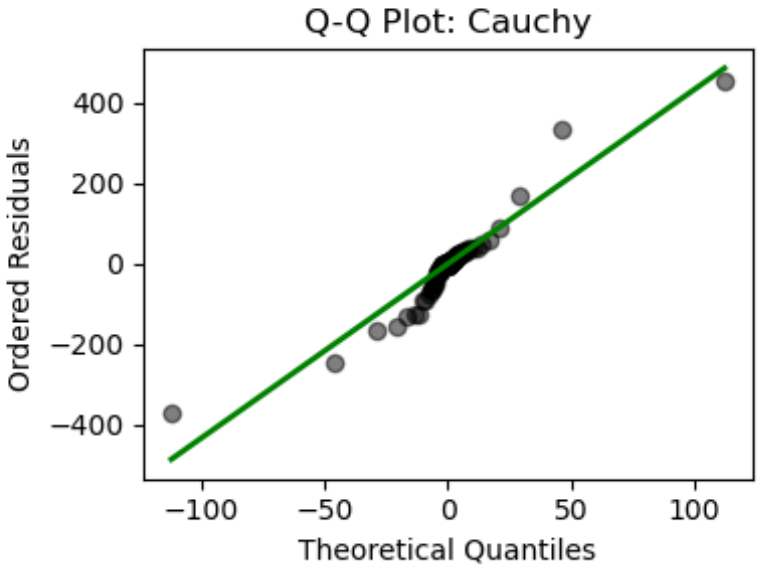


Distribution of Residuals







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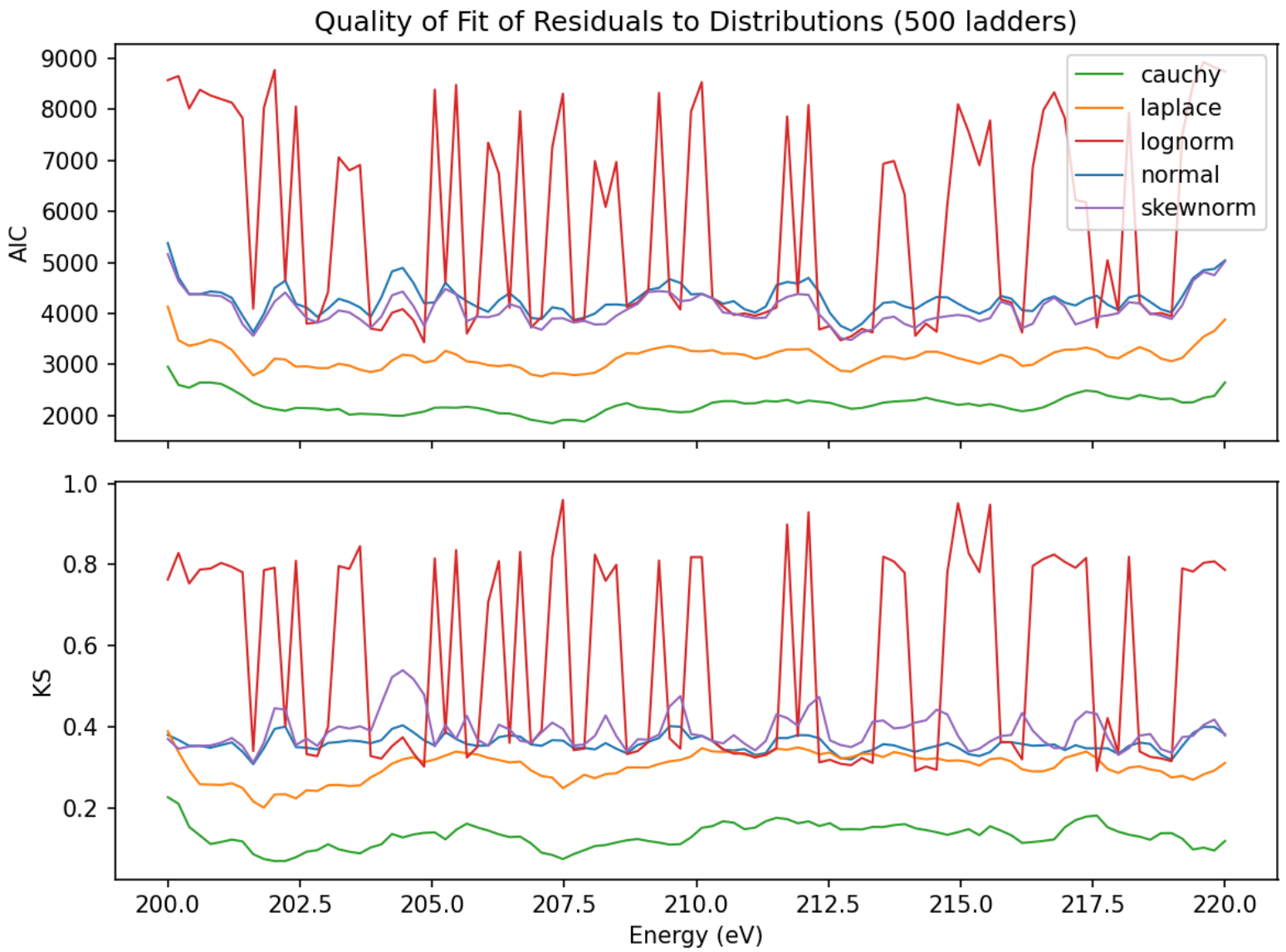
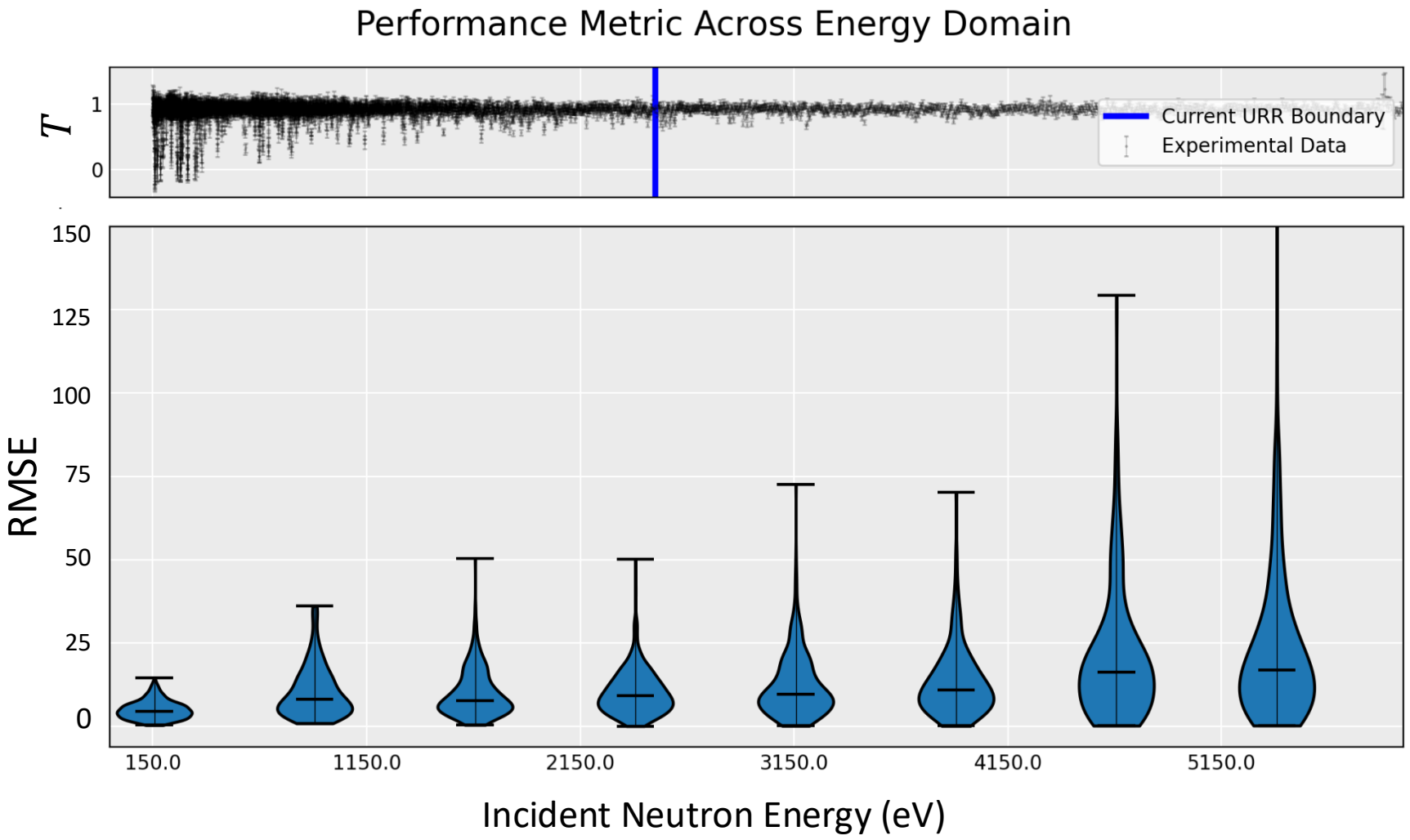
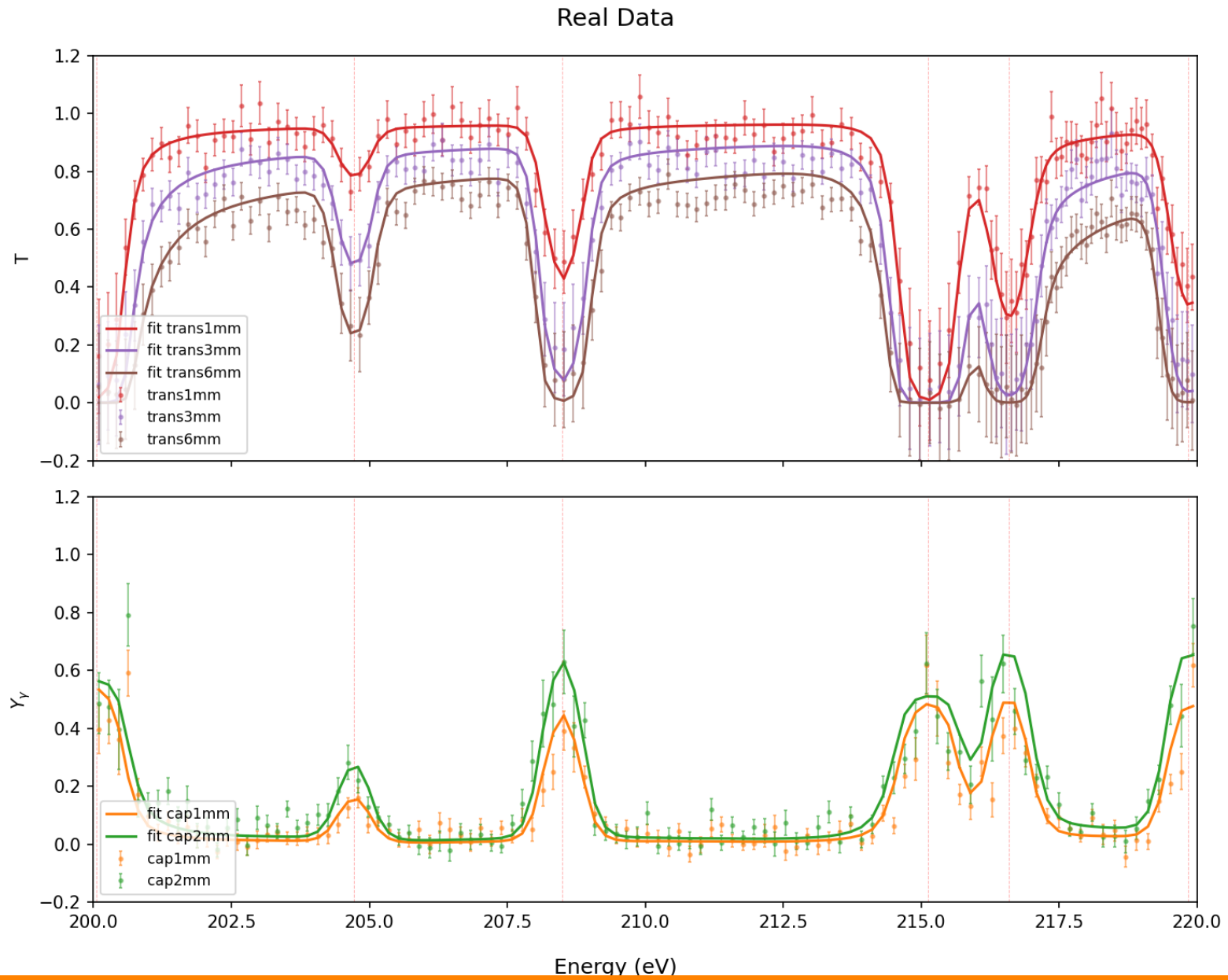



Performance Metric Across Energy Domain
T
1
0
Current URR Boundary
Experimental Data
RMSE
150
125
100
75
50
25
0
150.0
1150.0
2150.0
3150.0
4150.0
5150.0
Incident Neutron Energy (eV)

Real Data



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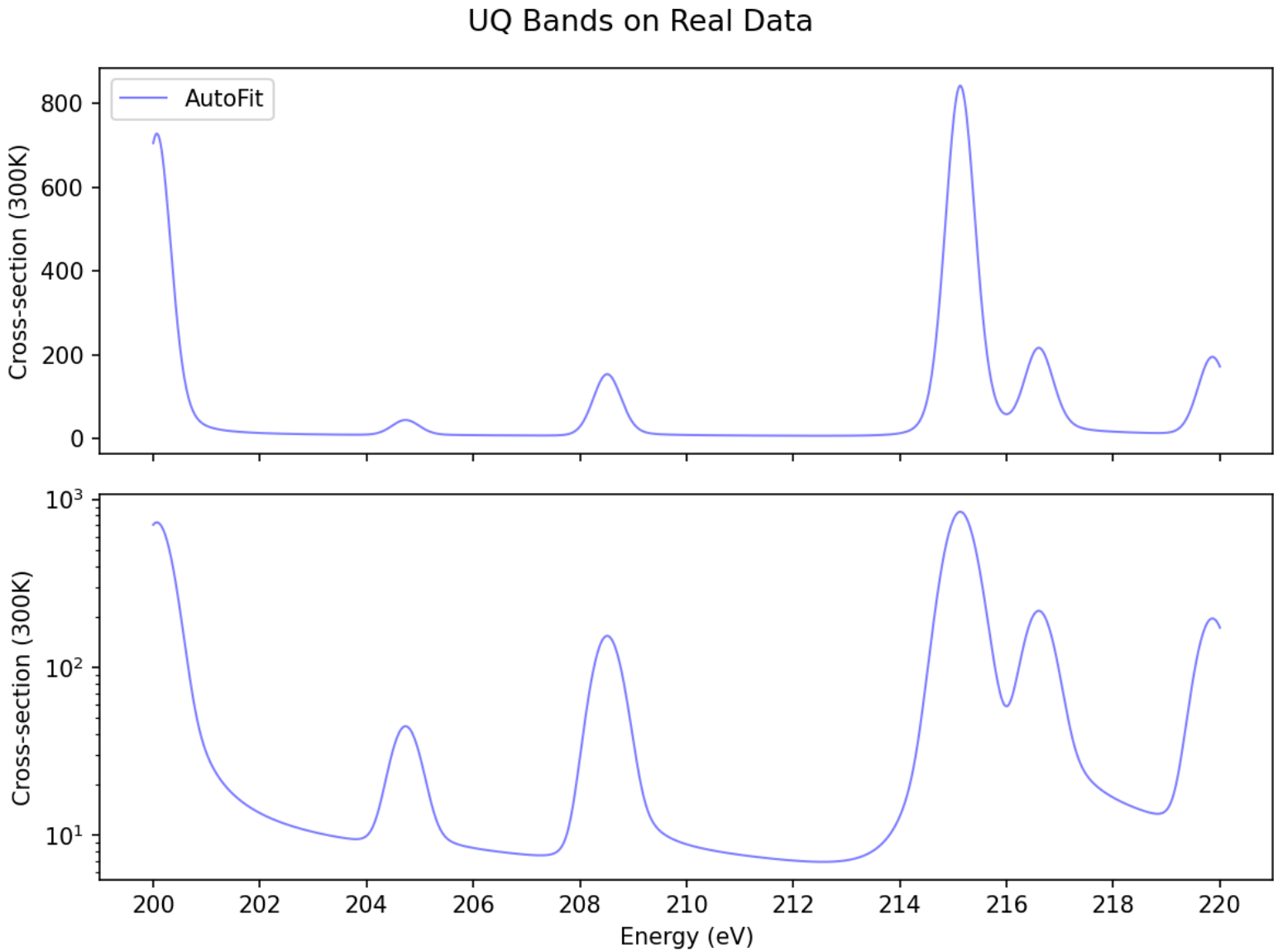

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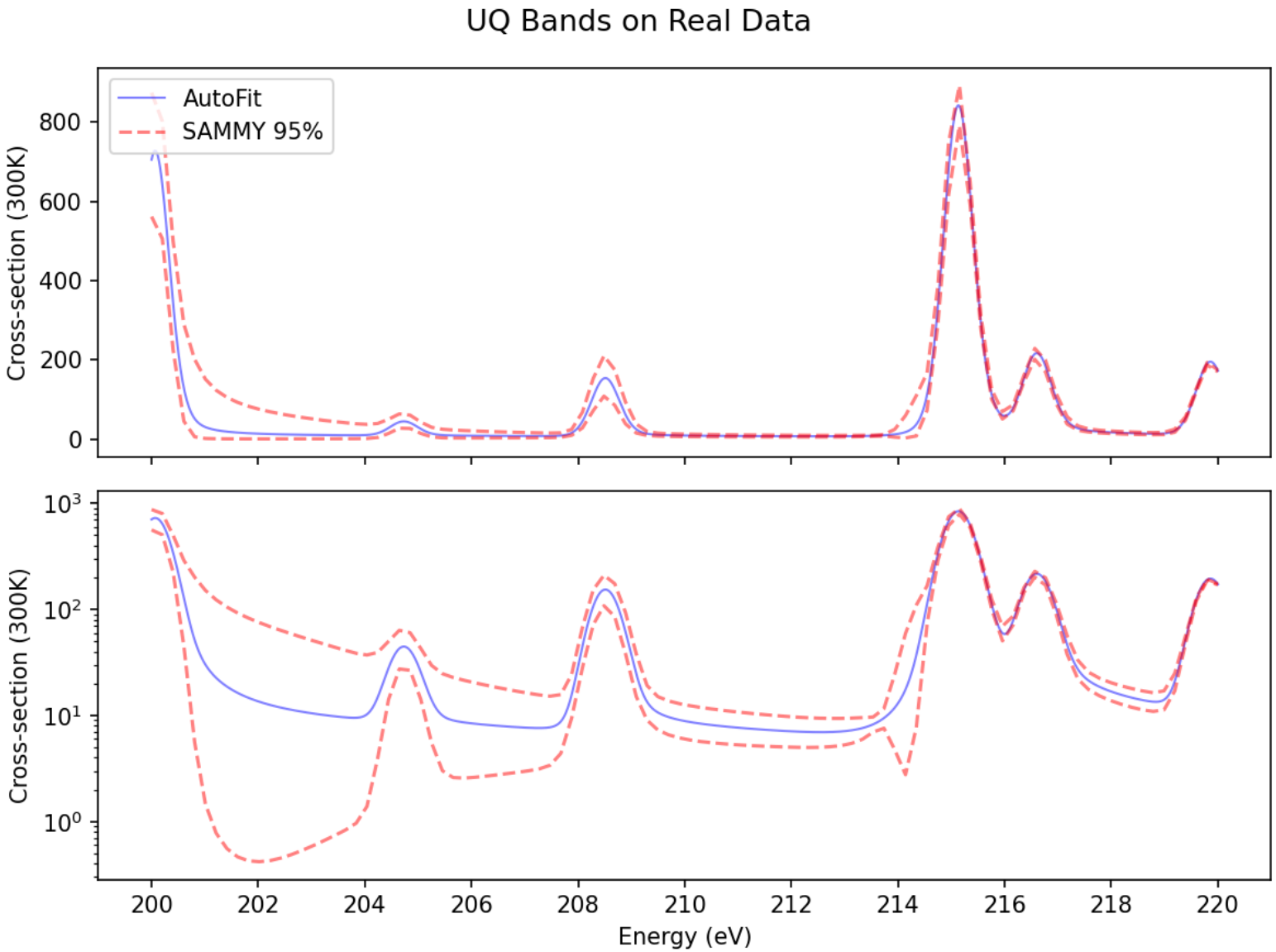

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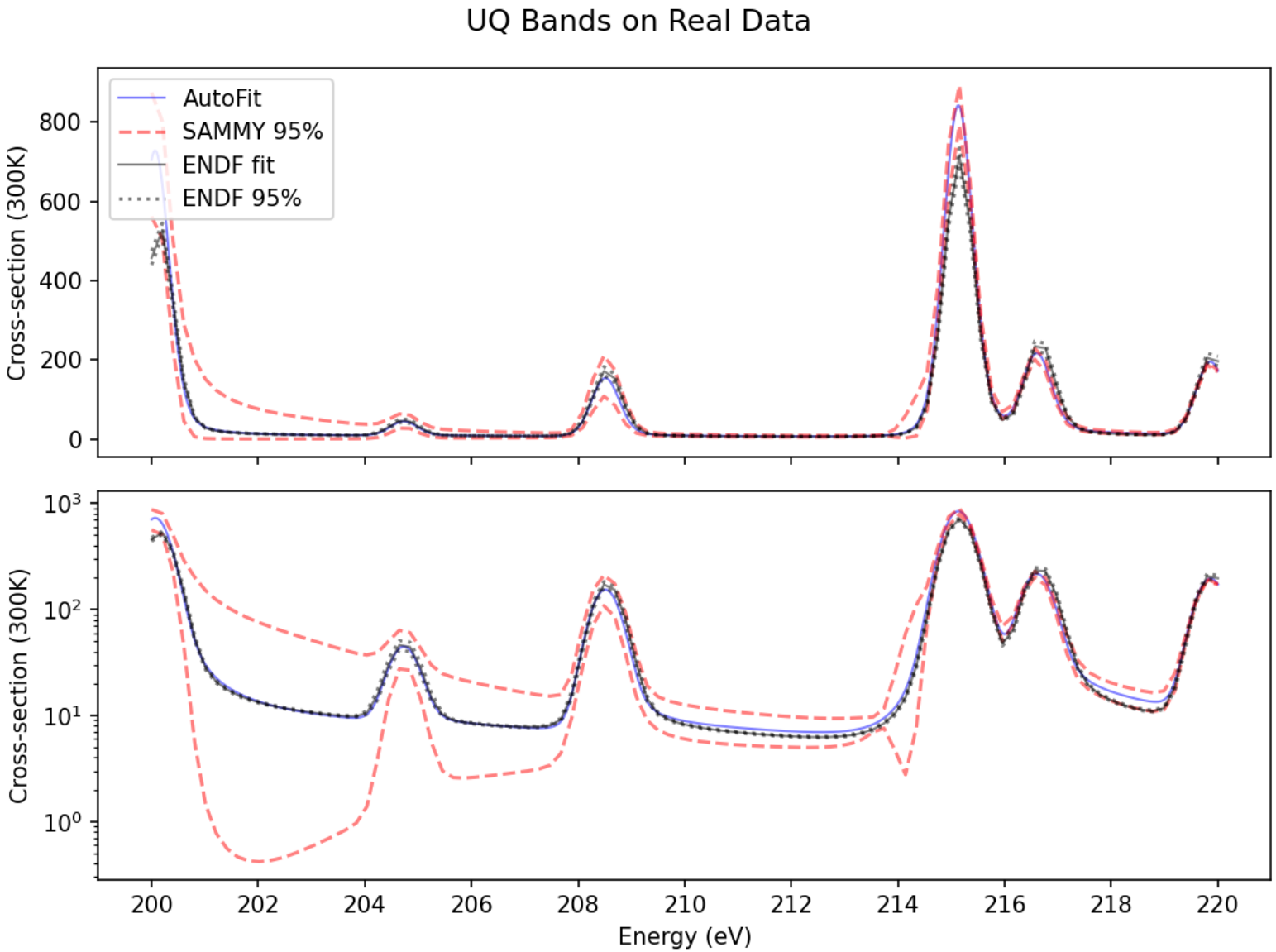
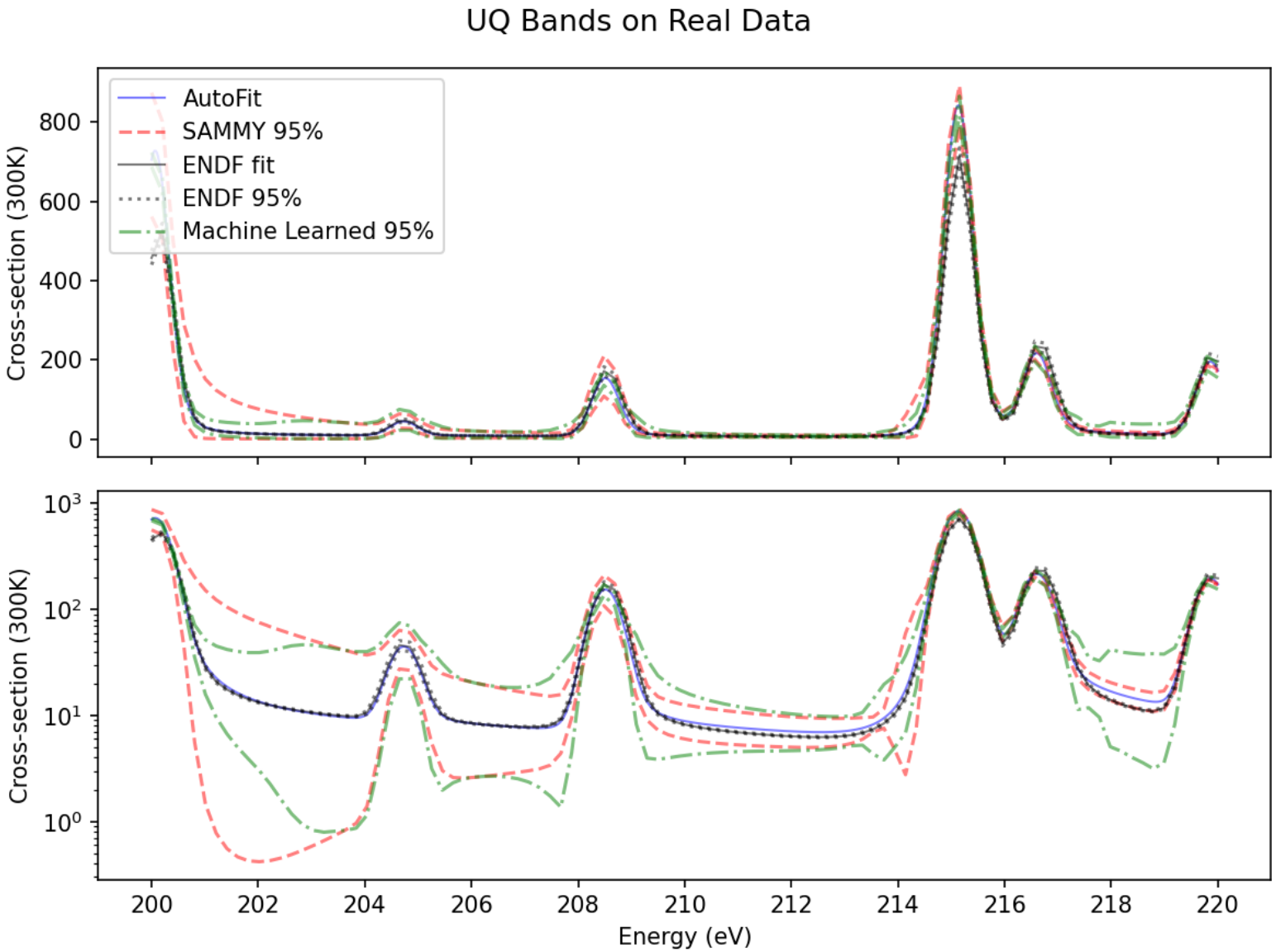


Real Data



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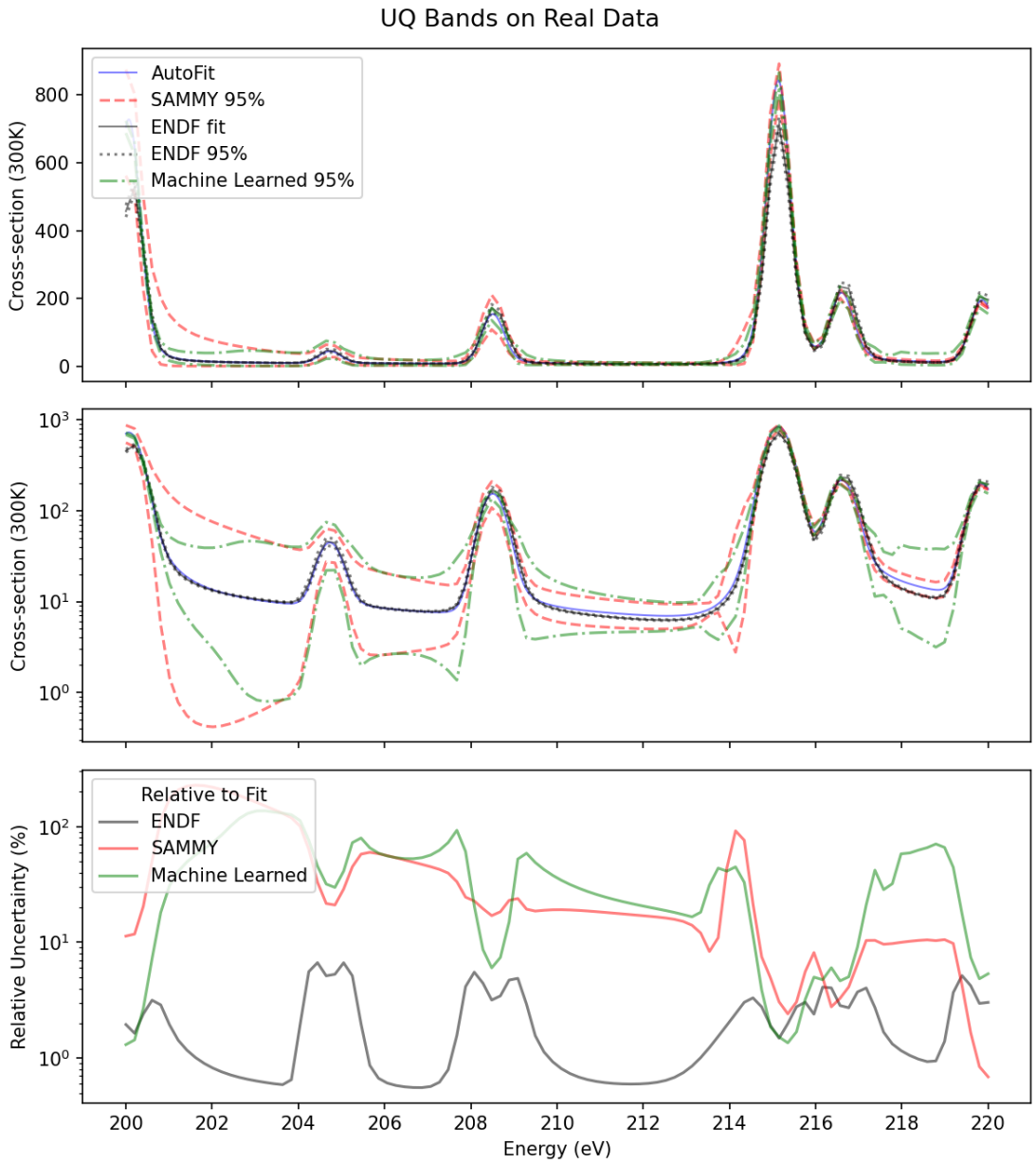


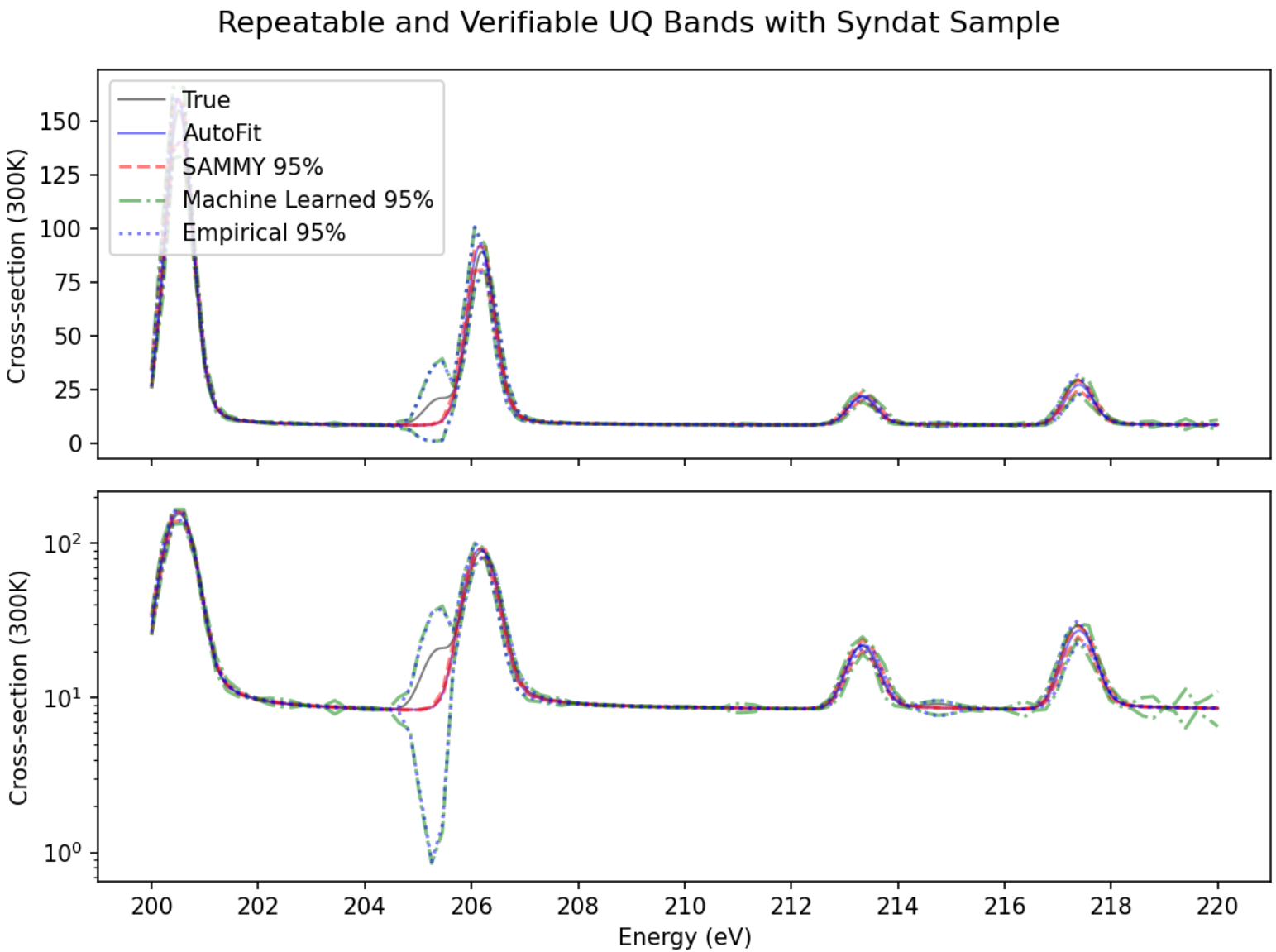
Conclusions

1. A train-then-test process using synthetic data allows us to verify the performance of any UQ approach.
2. Machine learning methods which combine SAMMY UQ output from higher-order models may produce more accurate UQ for cross-sections than standard SAMMY UQ.

Future work

- Identify best metric for evaluating a candidate UQ relative to empirical UQ.
- Further explore candidate models for improved UQ
- Develop process for stitching learned UQ across energy windows

Questions?



References I

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