Uncertainty quantification in R-matrix analyses using Bayesian methods

Daniel Phillips

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BAND Bayesian Analysis of Nuclear Dynamics

RESEARCH SUPPORTED BY THE DOE OFFICE OF SCIENCE, THE SSAP, AND THE NSF OAC

The Bayes-ics

Thomas Bayes (1701?-1761)

http://www.bayesian-inference.com

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Posterior

Model evidence

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Typically evaluated by MCMC sampling

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Posterior   Model evidence

Typically evaluated by MCMC sampling

Marginalization: $\mathrm{pr}(x|\mathrm{data},I) = \int dy\, \mathrm{pr}(x,y|\mathrm{data},I)$

Allows us to integrate out "nuisance" parameters, e.g., those associated with systematic uncertainties

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- Straightforward to introduce additional nuisance parameters to model experimental imperfections. Marginalizing over them includes impact of those imperfections on parameters and evaluated quantities

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Outline

- What is all this fuss about Bayesian methods? Why should I care?
- Bayesian R-matrix analysis of ^{3}He + ^{4}He→^{7}Be + γ and ^{3}He + ^{4}He elastic scattering

  Odell, Brune, DP, deBoer, Paneru,Frontiers in Physics (2022)
  Paneru, Brune Connolly, Odell, Poudel, DP, et al. Phys. Rev. C (to appear)

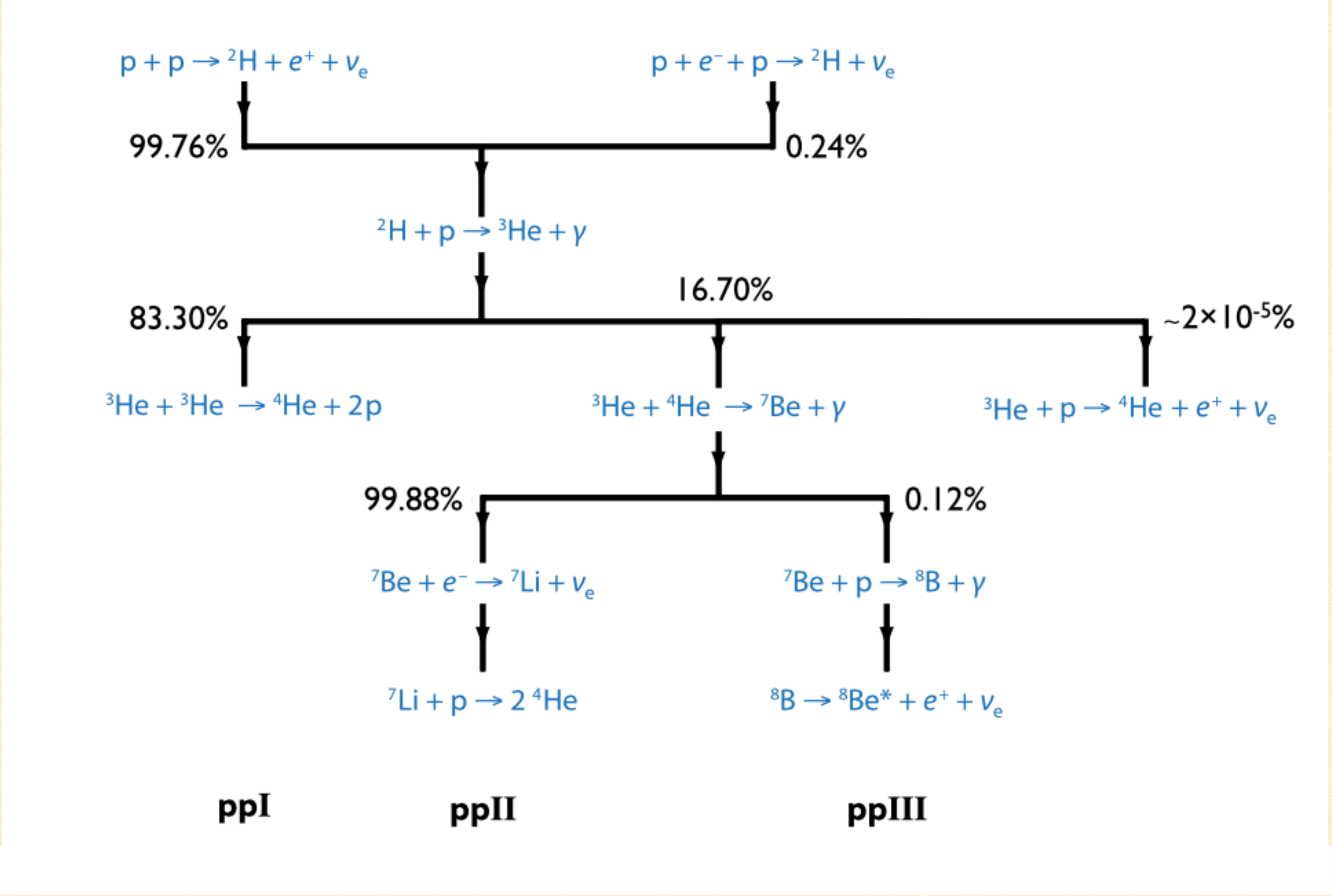
  - Set up
  - Experimental imperfections
  - Why the full posterior?
  - Error propagation
- Bayesian R-matrix analysis of dt fusion

  Odell, Brune, DP. Phys. Rev. C (2022)
- Summary and Future Work

Why is $^3He(^4He,\gamma)$ important?

Adelberger et al., Rev. Mod. Phys. 83, 195 (2011)

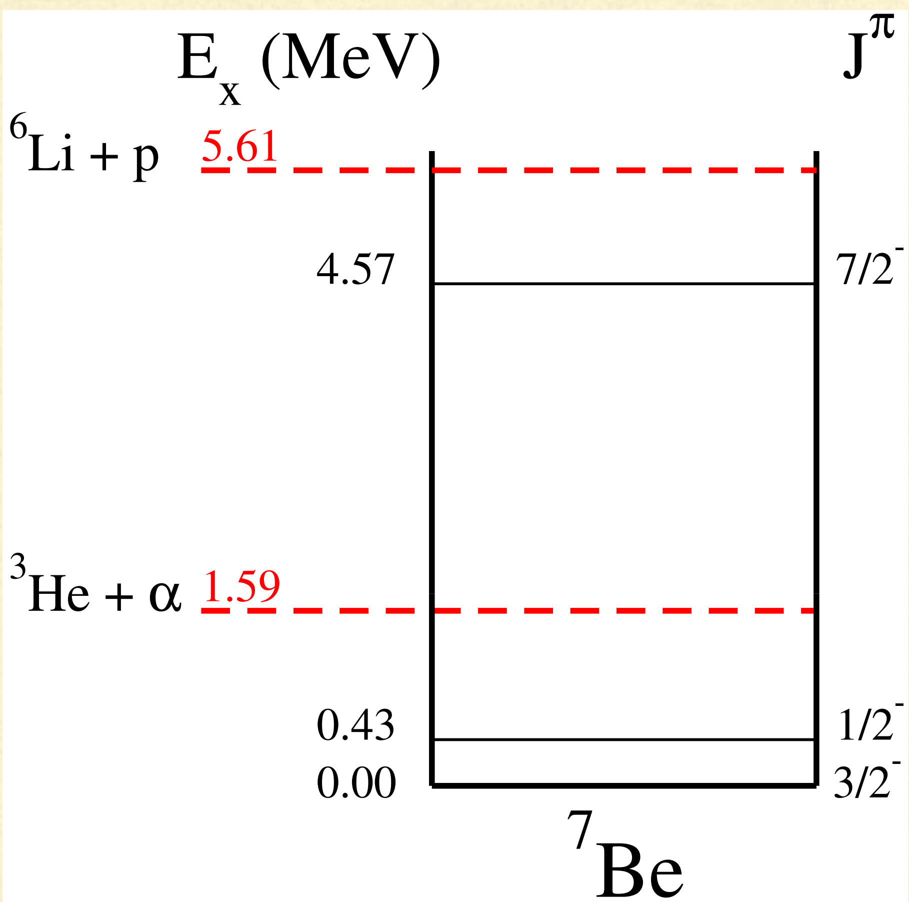
- Accurate knowledge of $^3He(^4He,\gamma)$ needed to reliably predict amount of ^7Be in the Sun
- Therefore key for prediction of ^8B solar neutrino flux
- BBN implications, but I will not discuss those here



Build an R-matrix model

Odell, Brune, DP, deBoer, Paneru, Frontiers in Physics (2022)

- Goal: describe scattering and capture data up to the p^{6}Li threshold
- 3/2- and 1/2- bound states with prior ranges for ANCs from 1 to 5 MeV



Background & resonance levels

	E (MeV)	Γ_α (MeV)
1/2-	21.6	[-200.200]
3/2-	21.6	[-100,100]
5/2-	7	[0,100]
7/2-	[2,10]	[0,10]
1/2+	14	[0,100]
3/2+	12	[0,100]
5/2+	12	[0,100]

Pick data sets

- 88 S-factor data
  - Seattle (S)
  - Weizmann
  - Luna (L)
  - Erna
  - Notre Dame
  - Atomki
- Plus 34 branching-ratio data

- Scattering data
  - SONIK*: 451 from 0.385 to 3.127 MeV
  - Barnard: 646 from 1.49 to 3.27 MeV

* Paneru et al., arXiv:2211.14641, Phys. Rev. C (in press)

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Two analyses:

Capture + SONIK

Capture + SONIK + Barnard

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- Publicly available Python code

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- BAND Framework v0.2

  bandframework.github.io
- AZURE2 must be installed
- User specifies R-matrix model & data set in AZURE2
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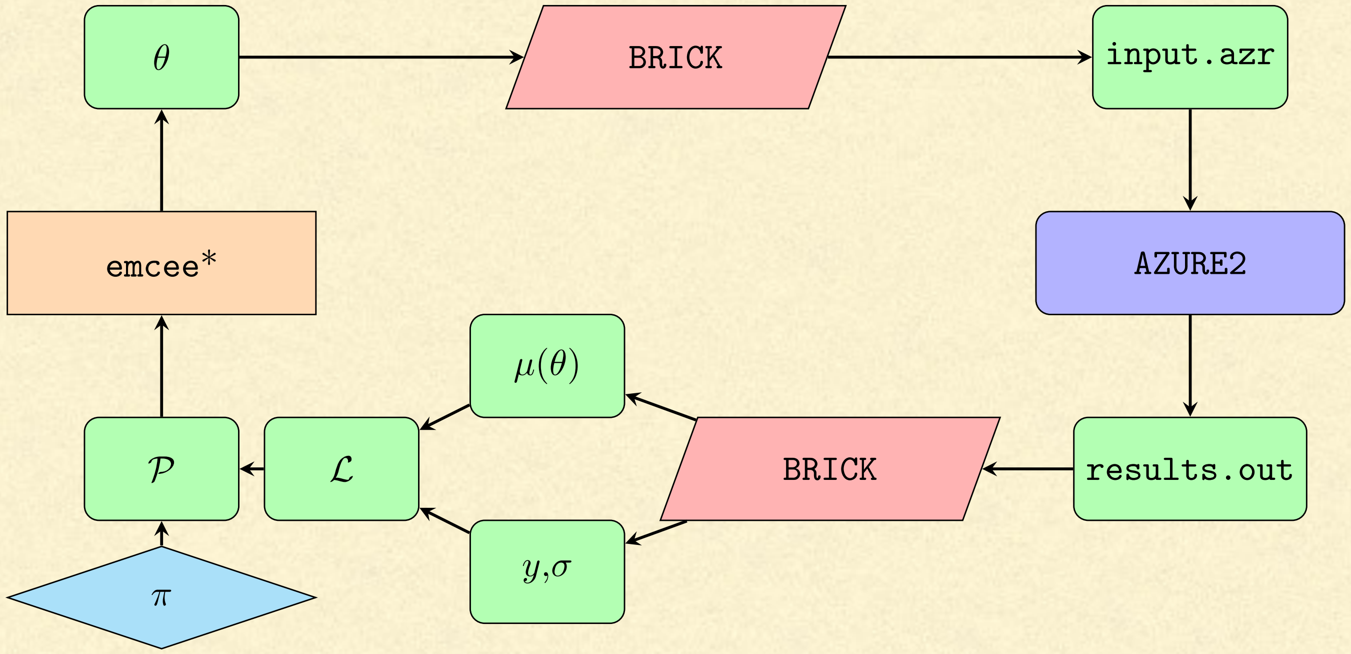

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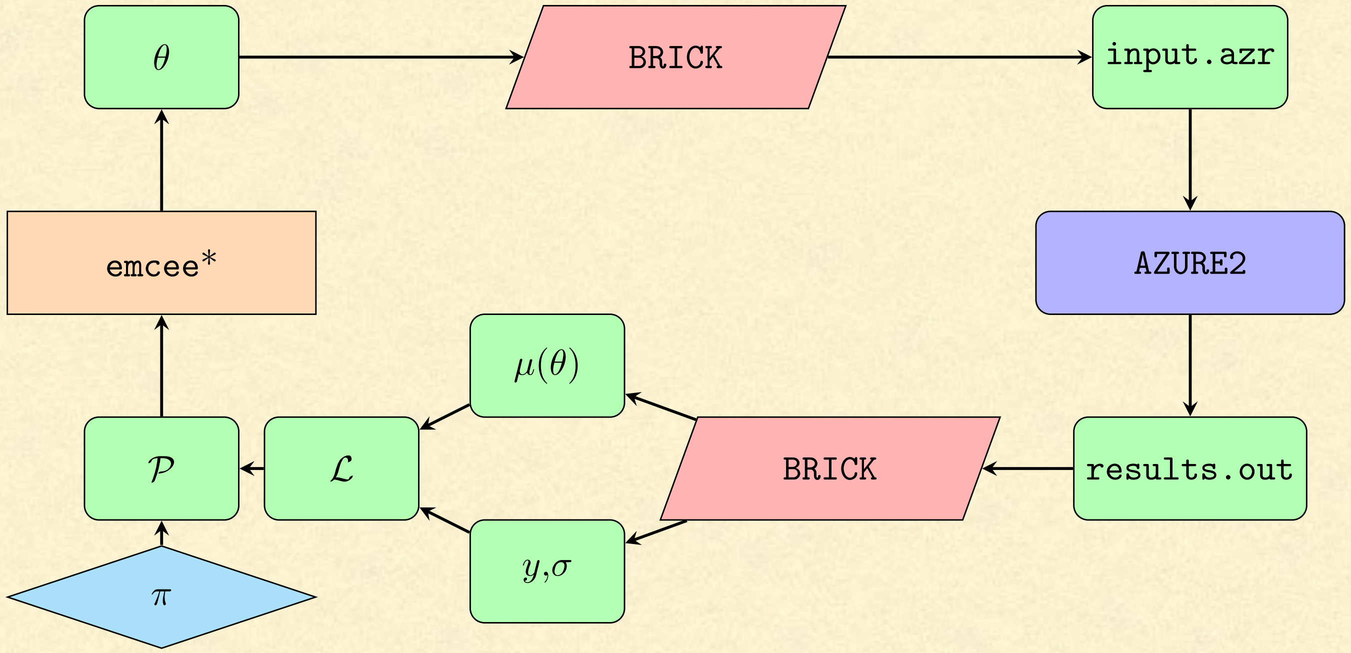

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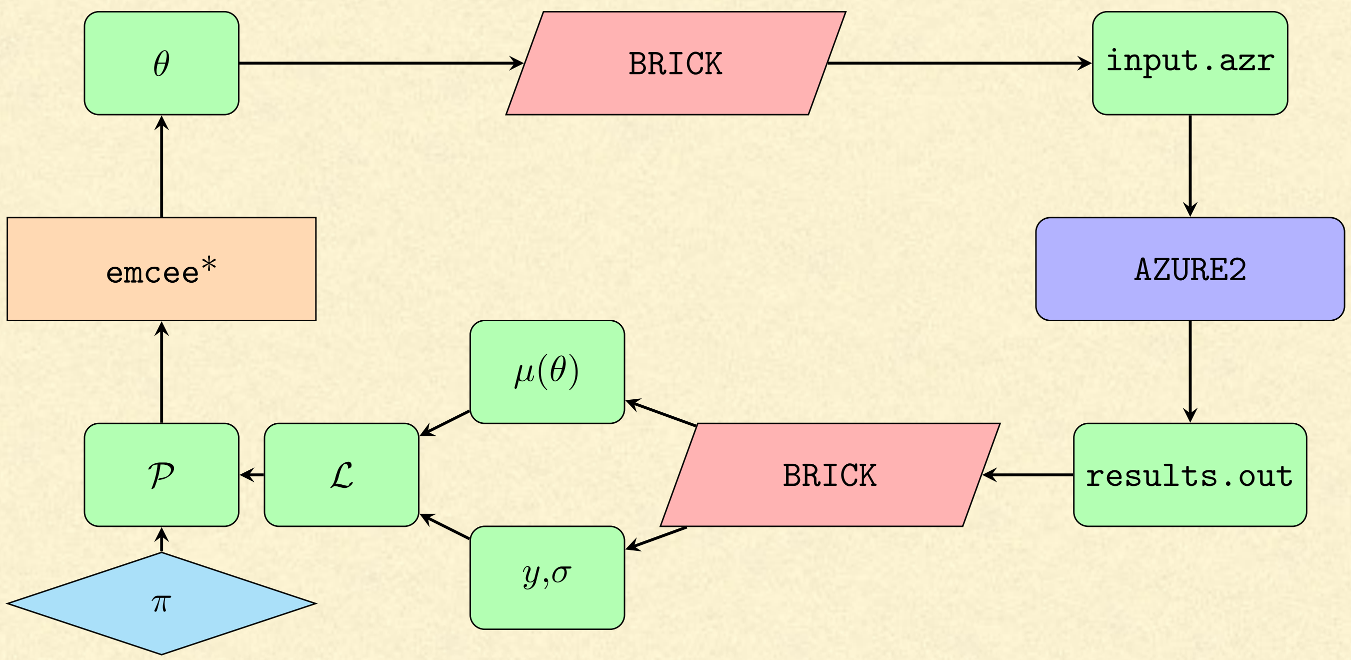

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Data

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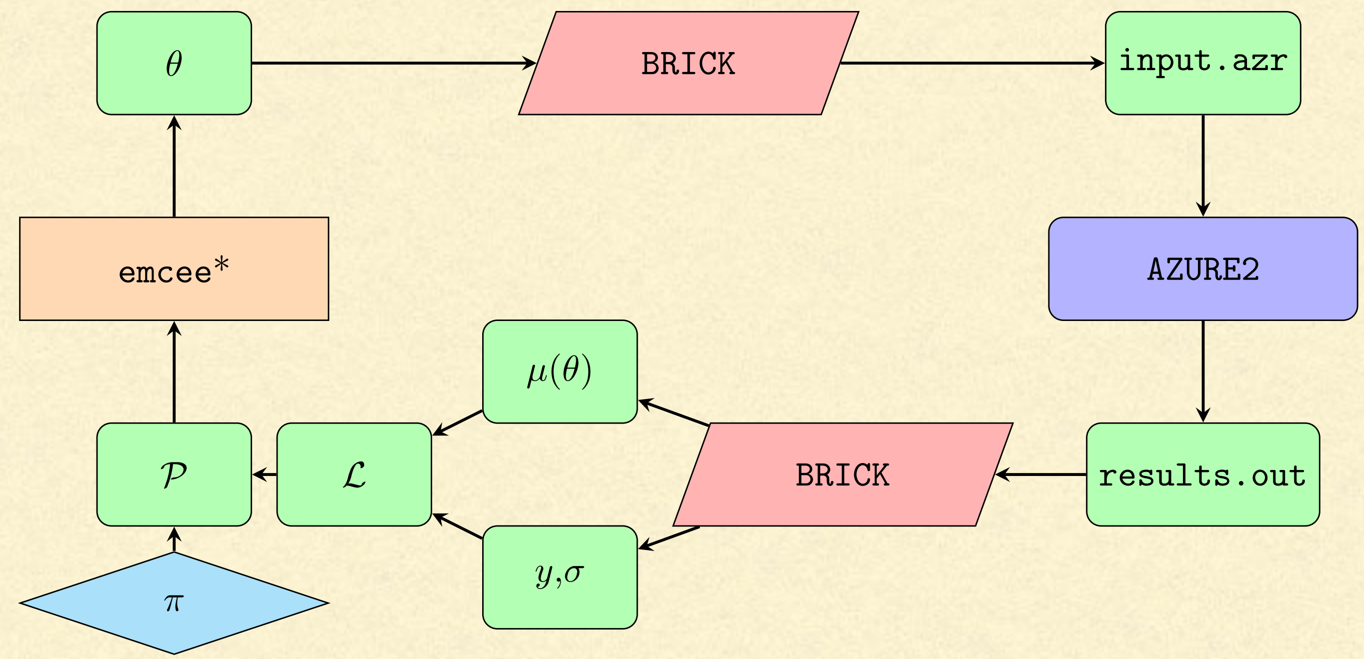

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R-matrix number

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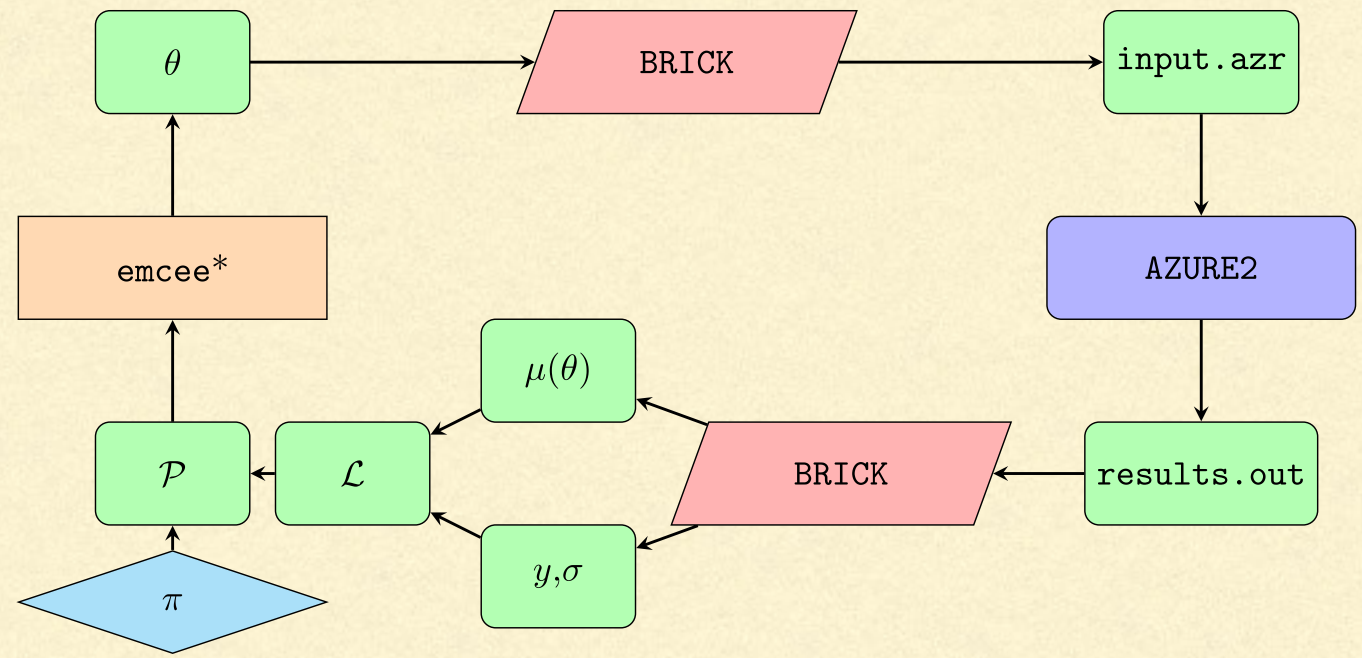

Data normalization

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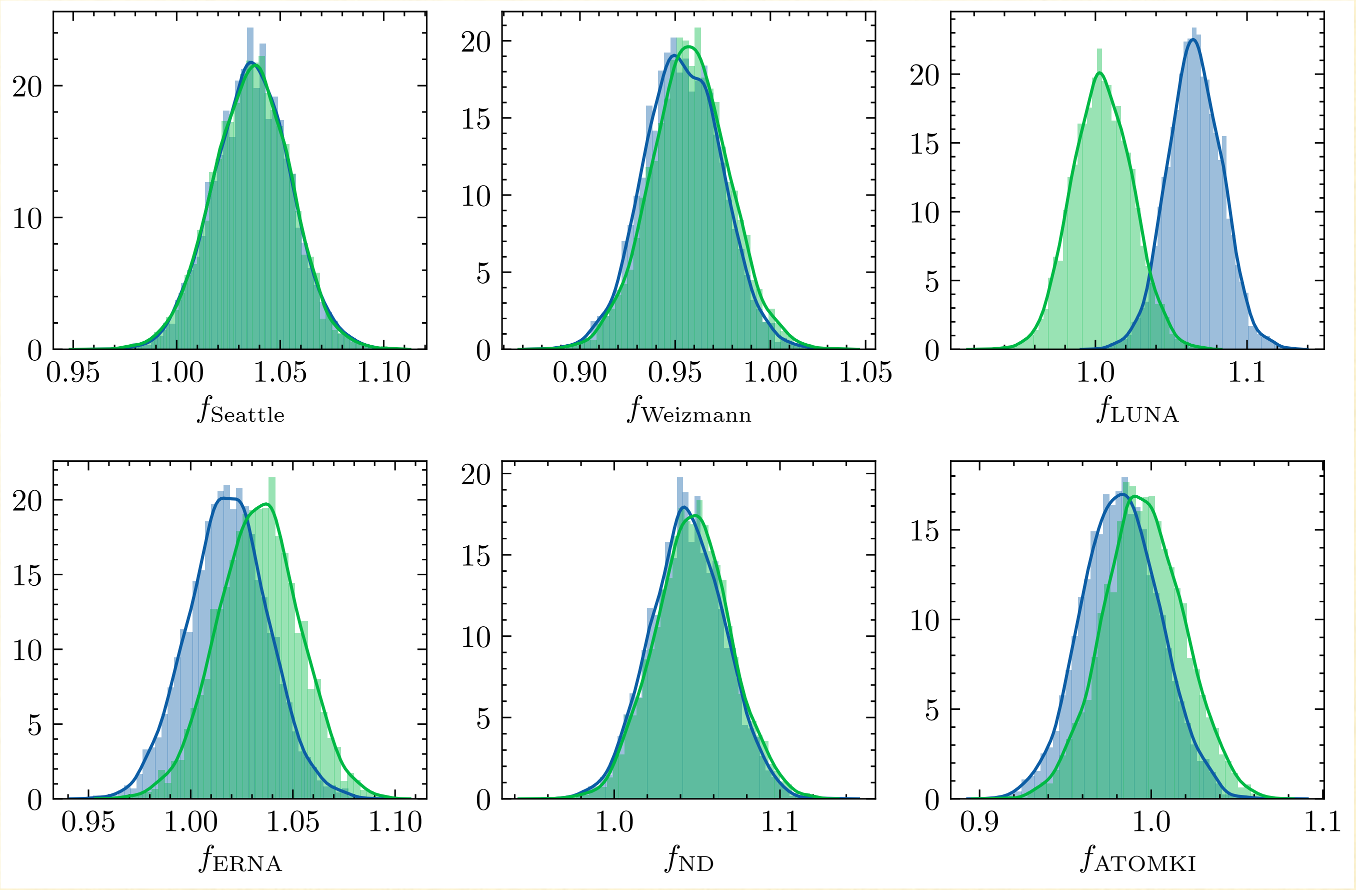
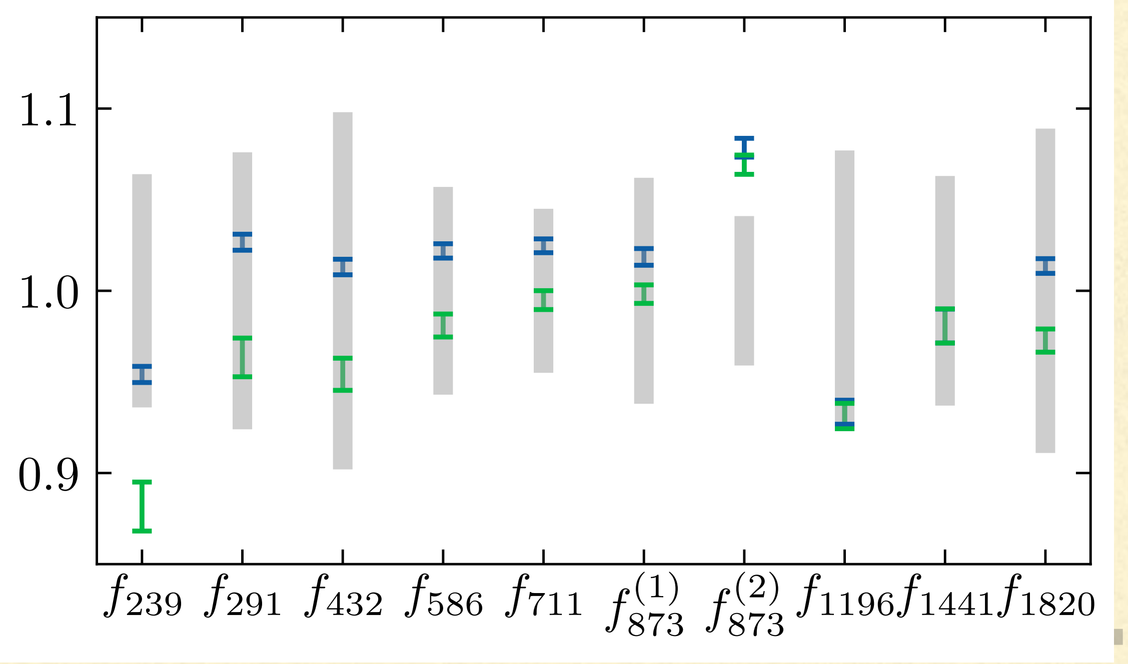
Modeling of normalization uncertainties

- Analysis includes common-mode errors for all data sets, implemented by factor f_α to avoid d'Agostini bias
- For SONIK data set this normalization factor is assigned for each beam energy
- Almost all normalizations come out inside quoted CMEs, all are within 2*CME, apart from LUNA in CSB analysis
- "Dialogue with the data"



CS

CSB



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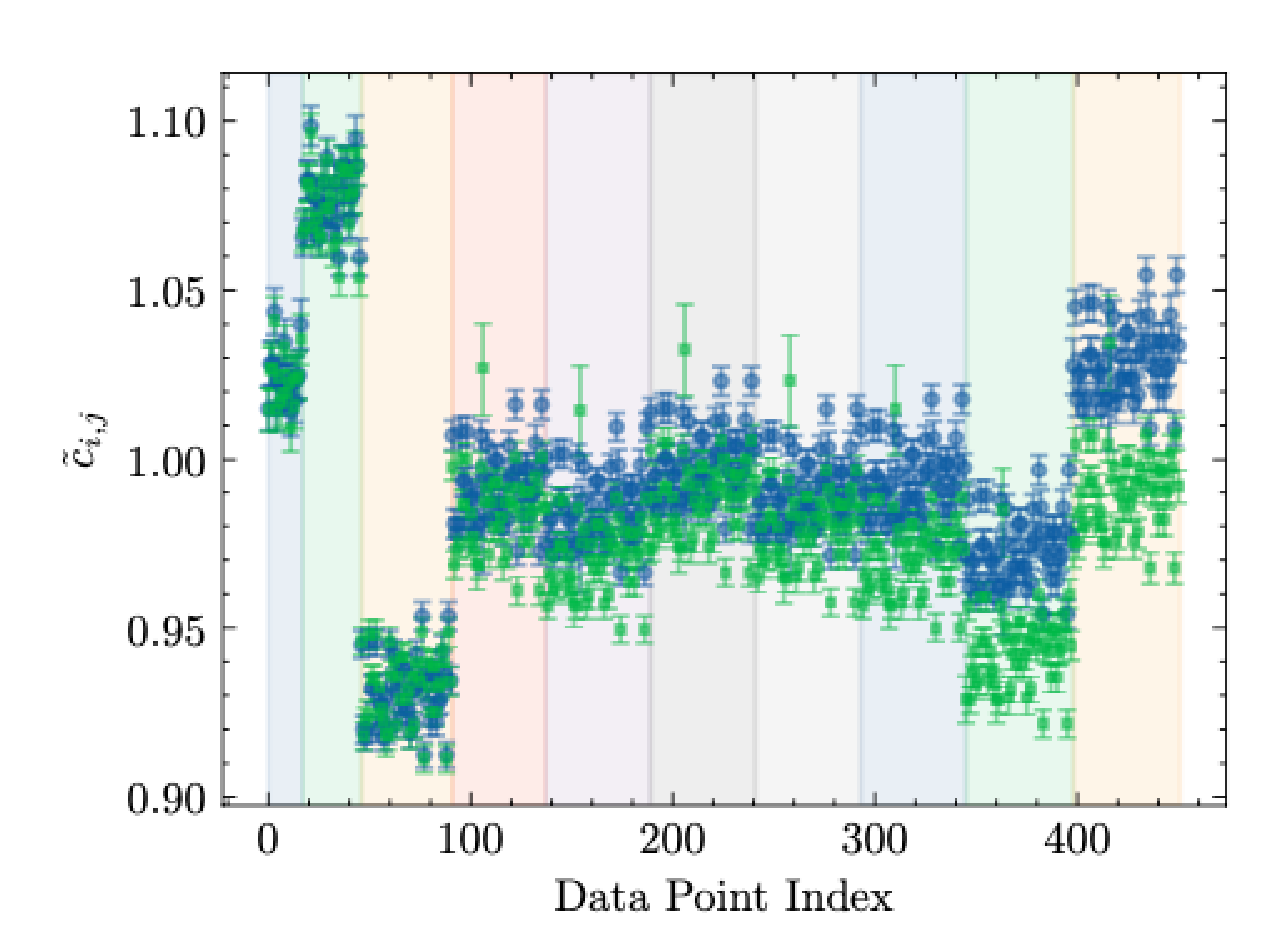

$$y_{\rm exp} = f_{\rm SONIK} f_E f_{\rm det} y_{\rm R} + \delta y_{\rm exp}$$

$$\tilde{c}_{i,j} = f_E f_{\rm det}$$

Green: R-matrix
Blue: EFT

Beam energy shift

Beam energy shift

- Shift energy of Barnard data set by a constant to account for possible miscalibration of beam energy: $E \to E + \Delta$. Prior a Gaussian with standard deviation 40 keV←information in paper

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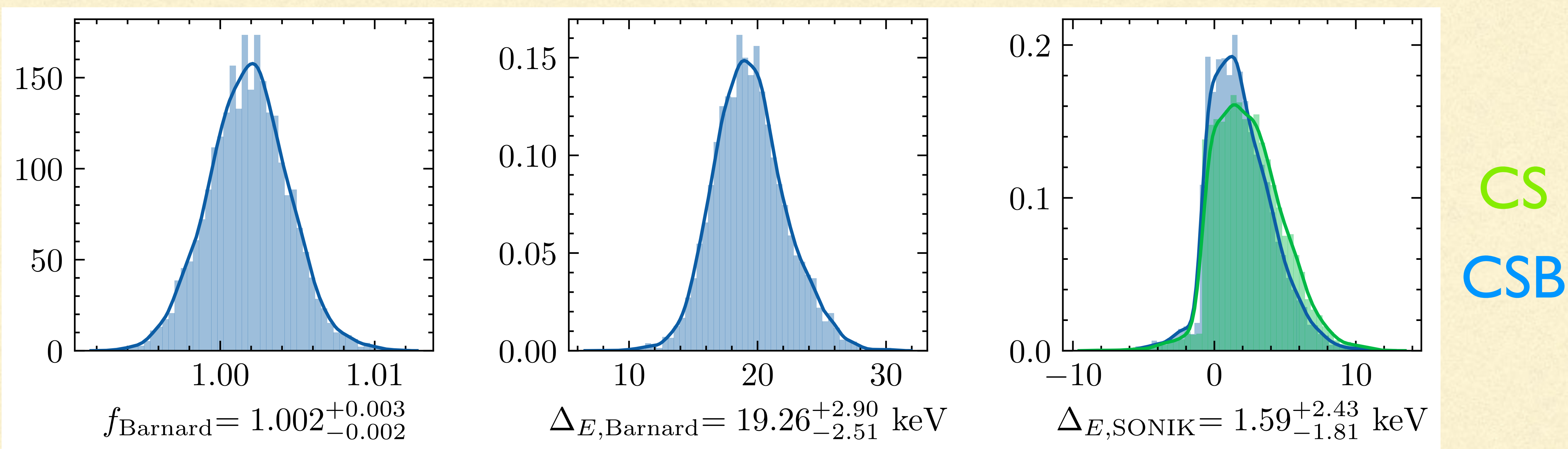

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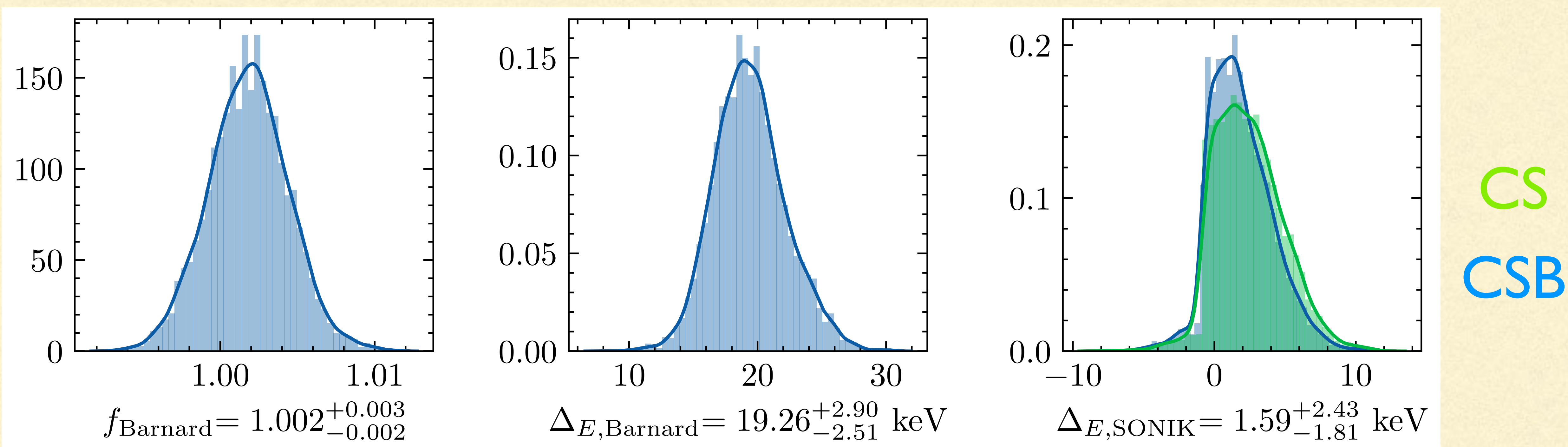
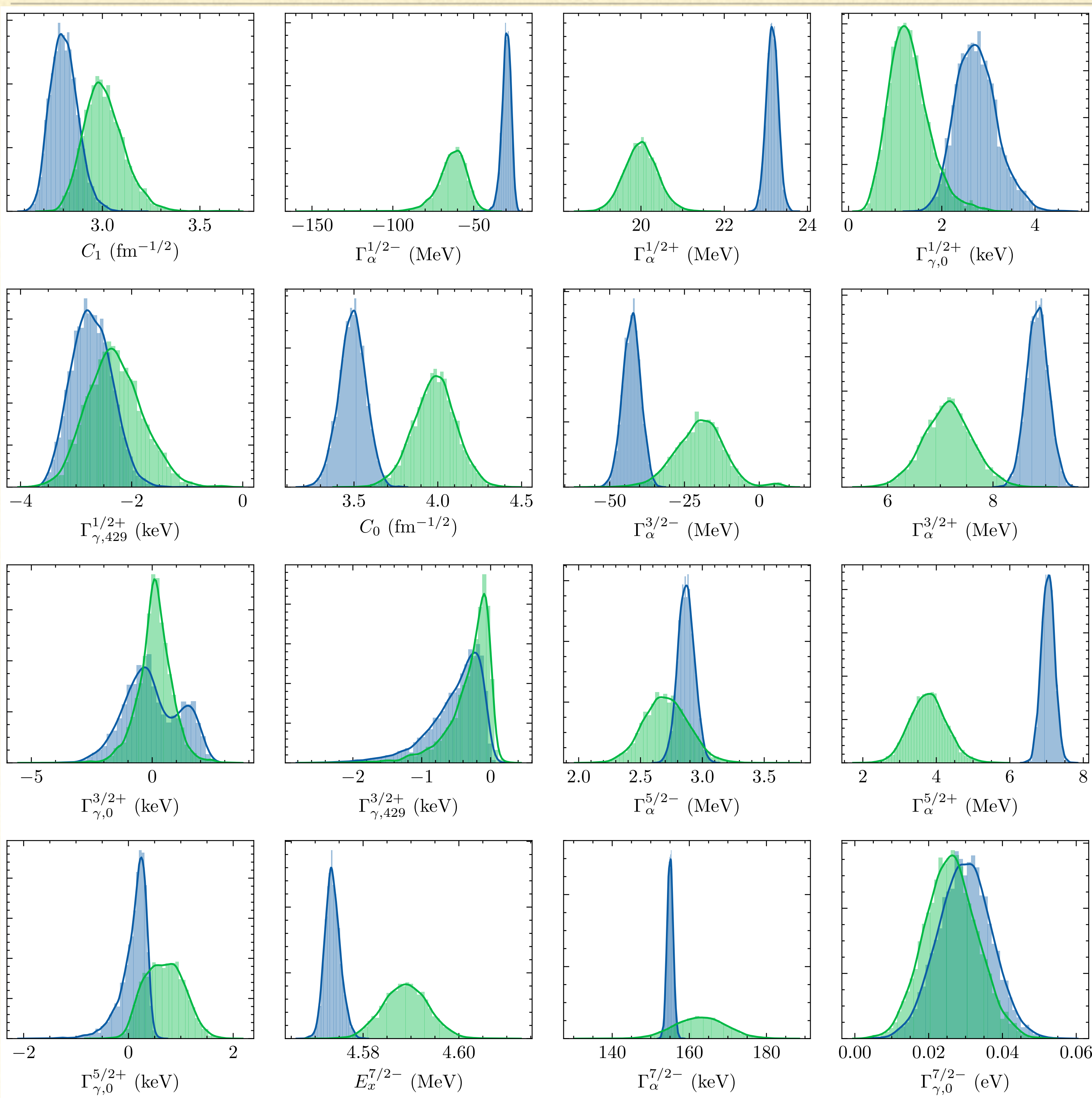


- No significant change in $\vec{\theta}_{\text{Barnard}}$ due to this though

Posteriors for R-matrix parameters



Capture + SONIK

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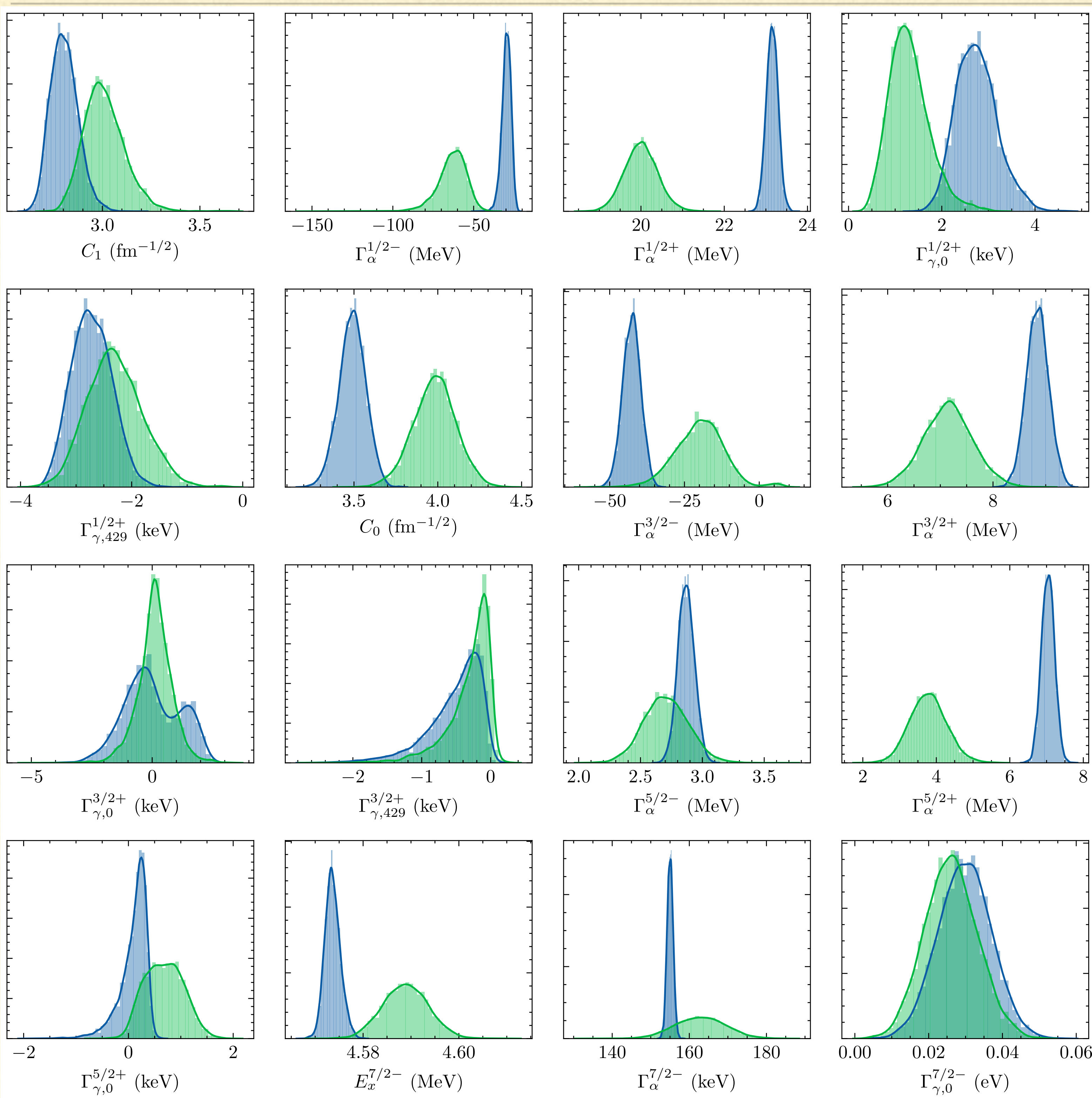

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Notable points:

- ANCs
- $\Gamma_\alpha^{7/2-}$
- Non-Gaussianity

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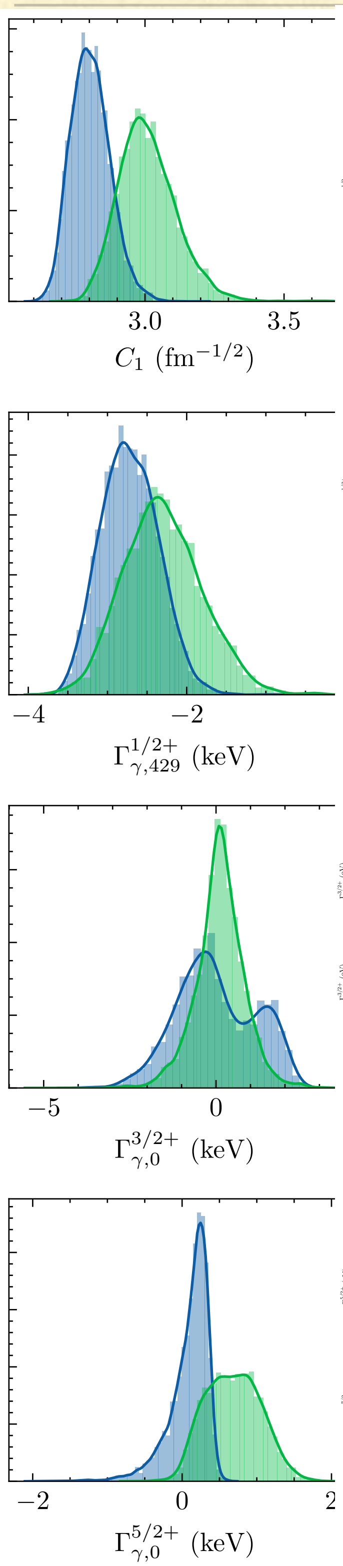

Access to all covariance information

re + SONIK

SONIK + Barnard

ble points:

Cs

2–

n-Gaussianity

But why didn’t you just use MINUIT?

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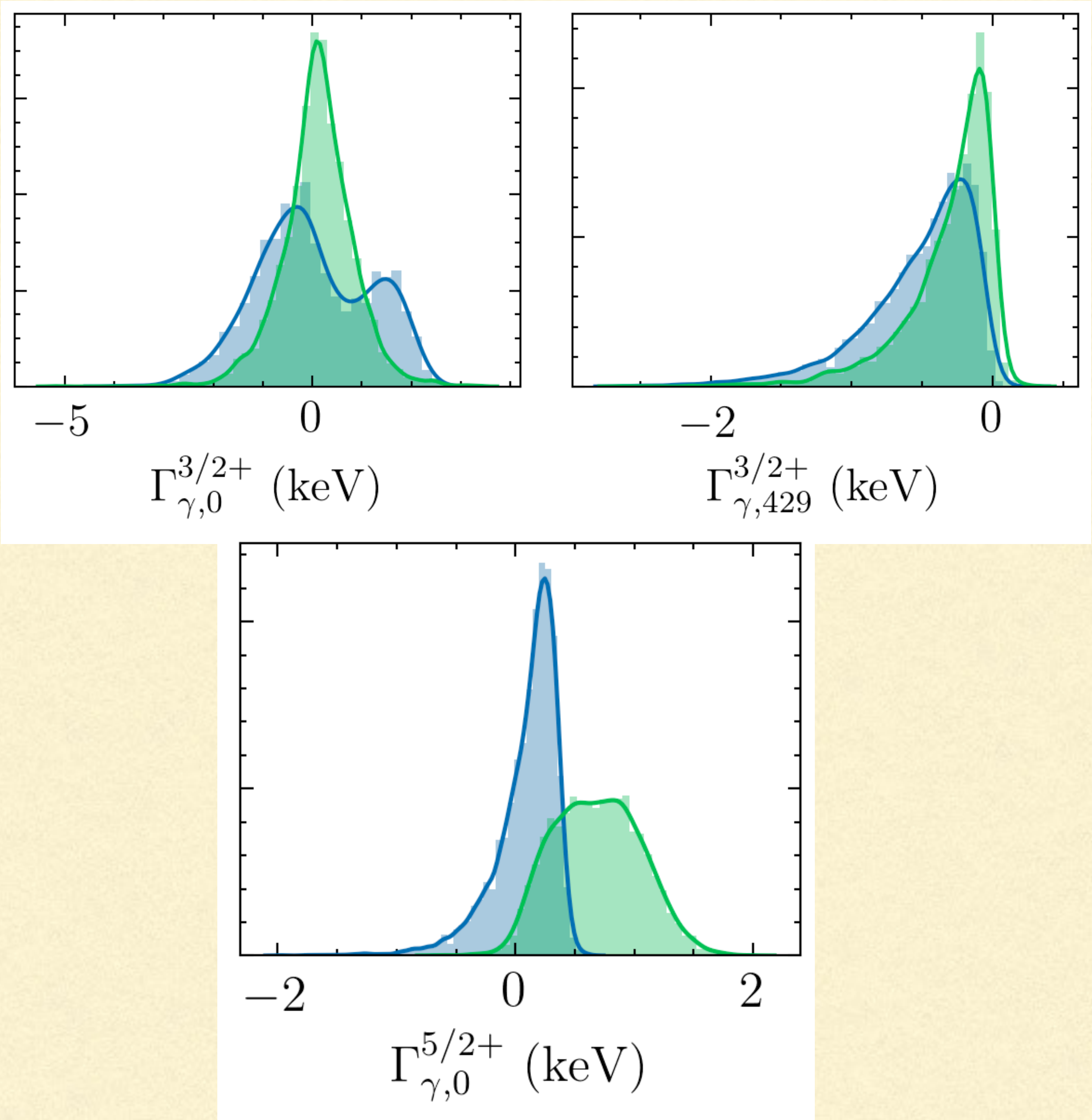
- Diagnose non-Gaussianity



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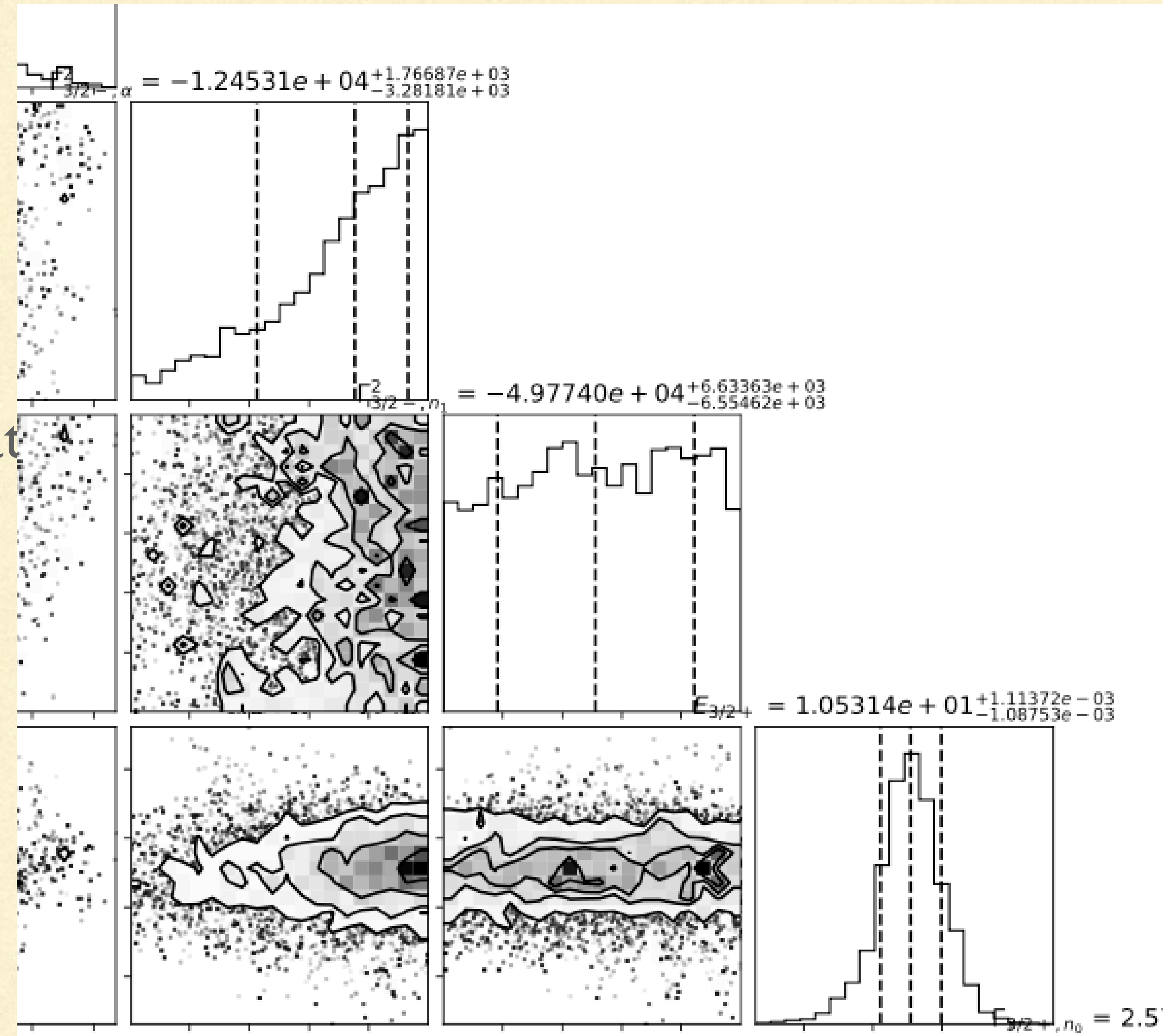

^{13}C(α,n), courtesy James deBoer

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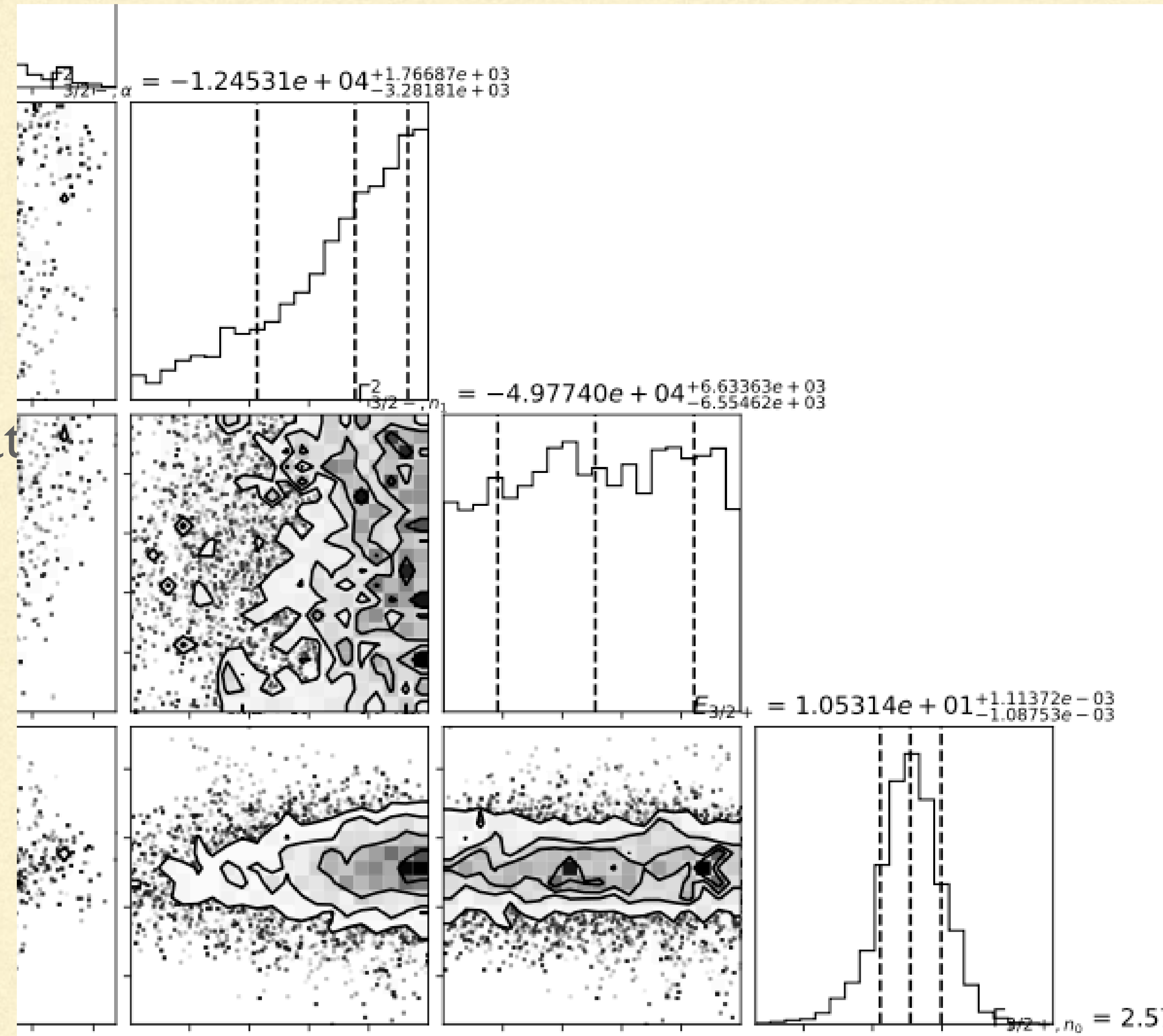

$^{13}C(\alpha,n)$, courtesy James deBoer

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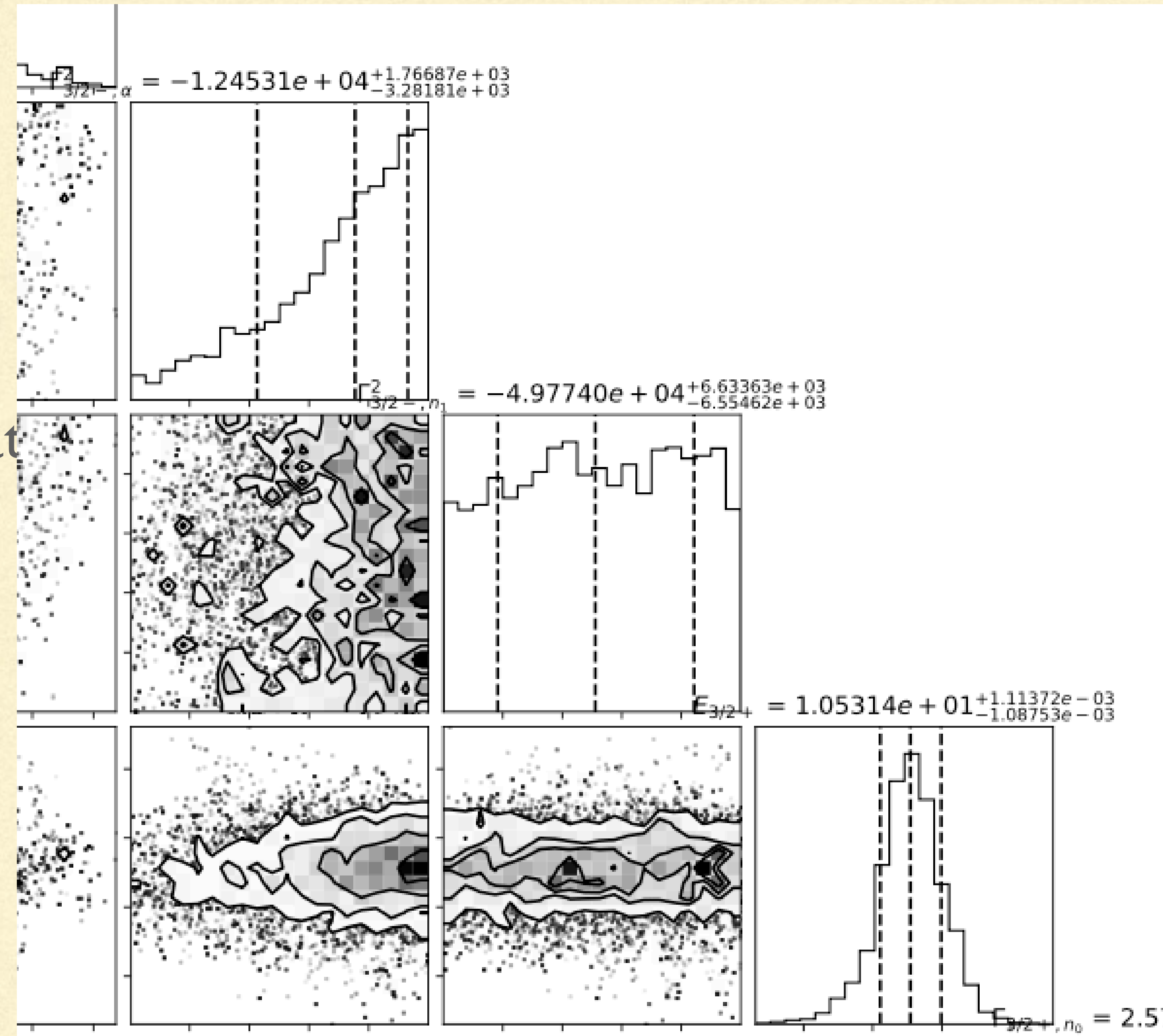
- (Note that it’s also clear when prior is affecting shape of posterior.)
- Also, error propagation….



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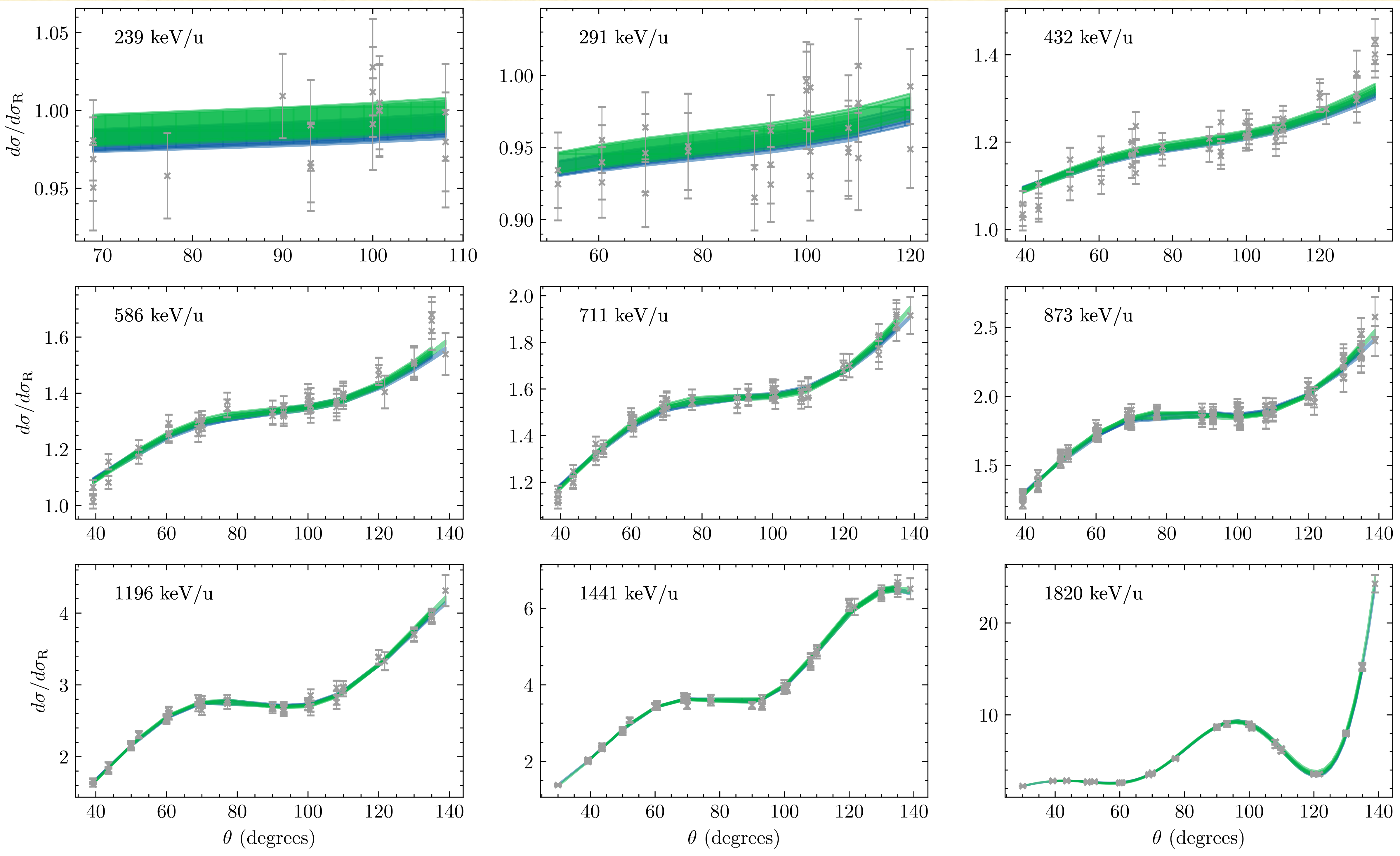
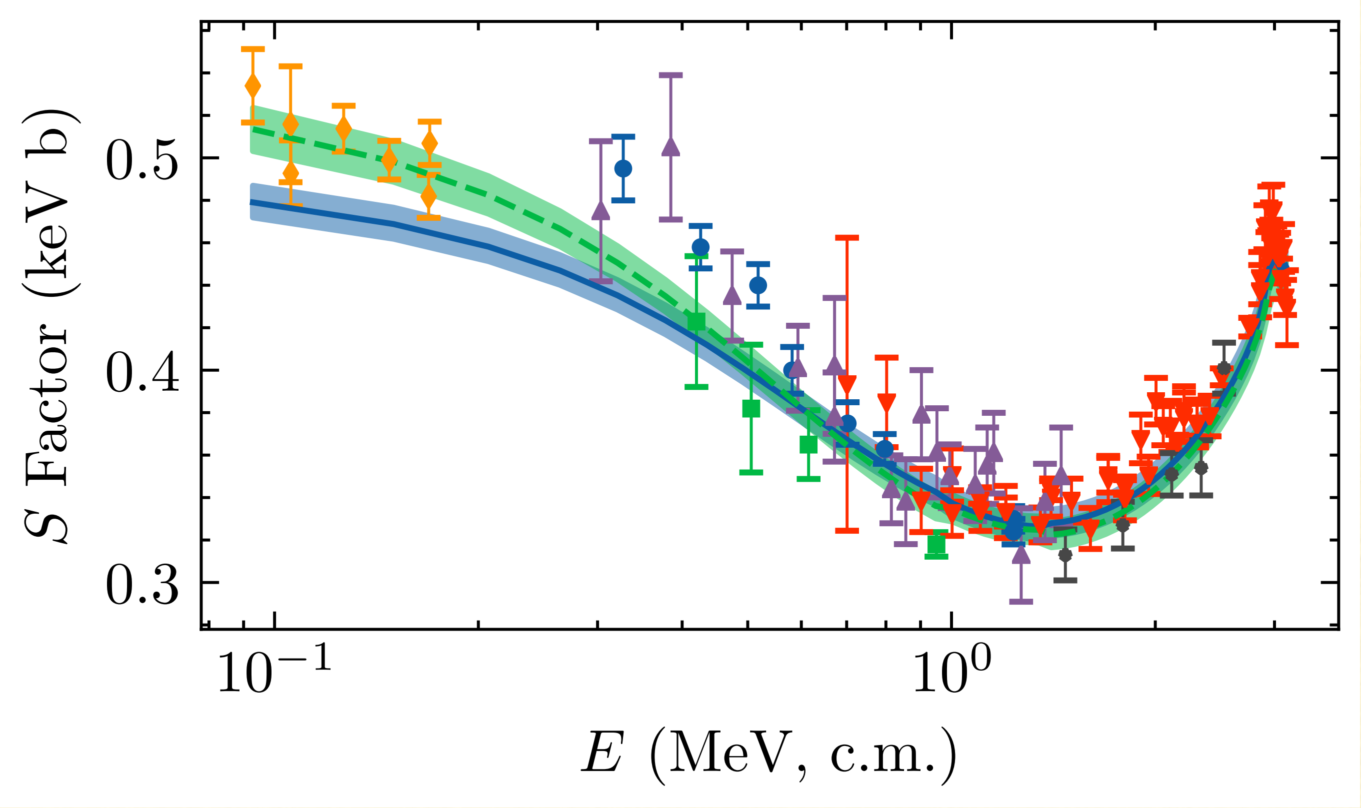
Speaking of which: SONIK data looks good



What about S-factor at solar energies?



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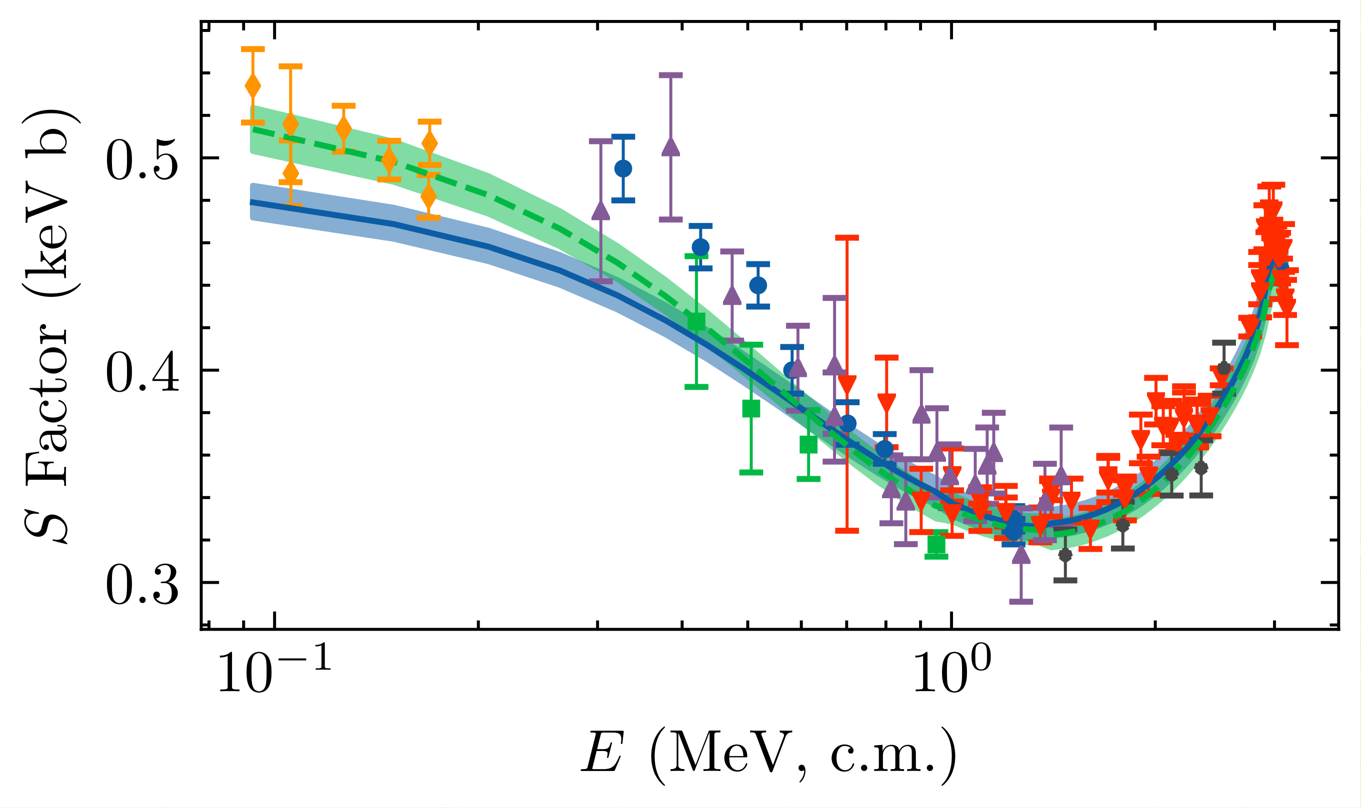

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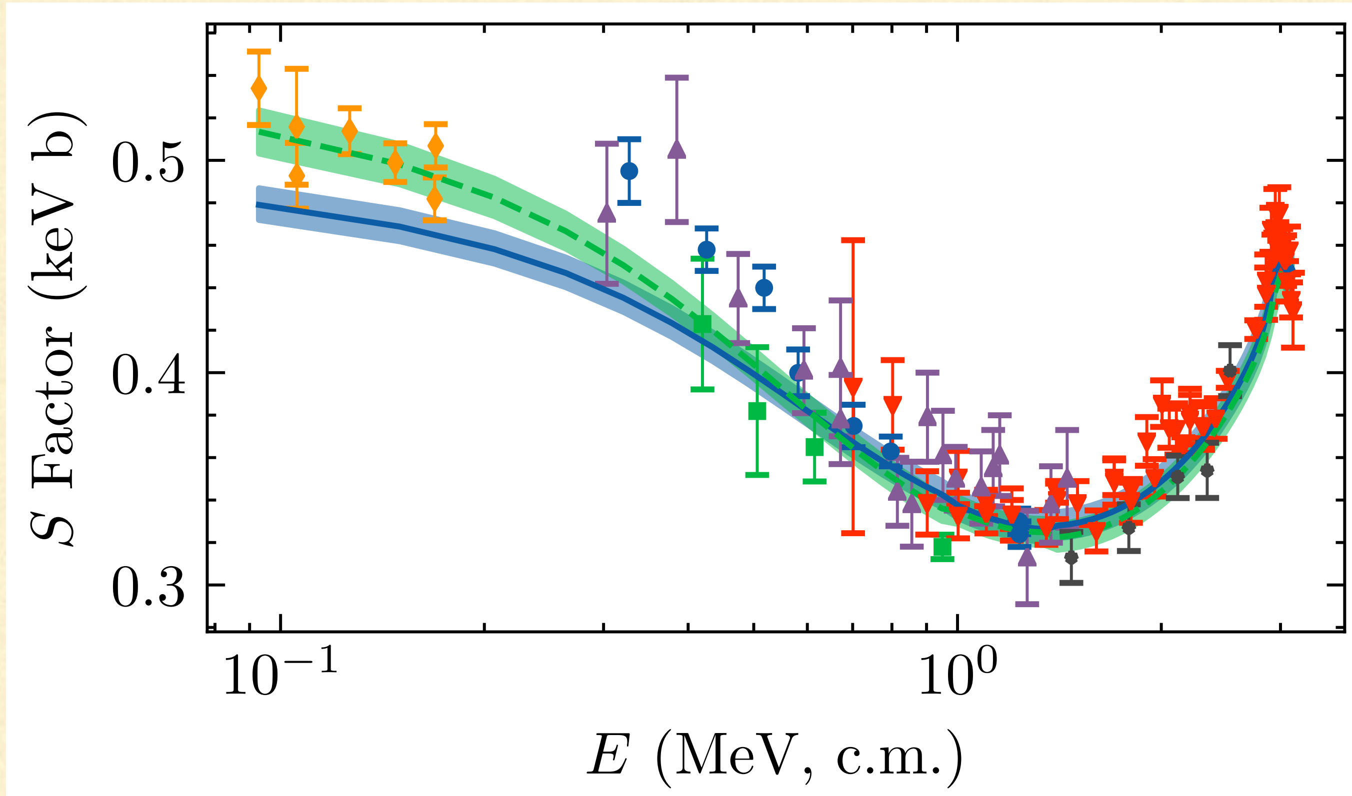

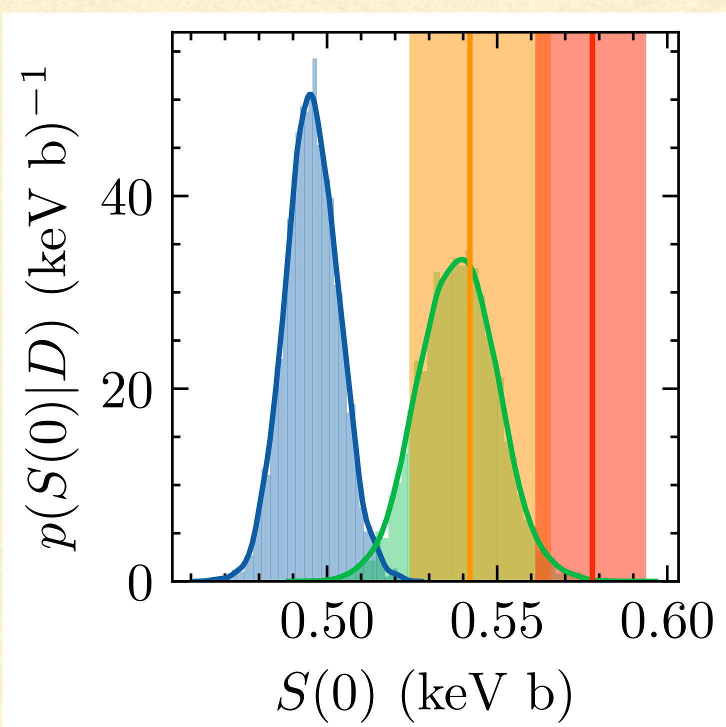

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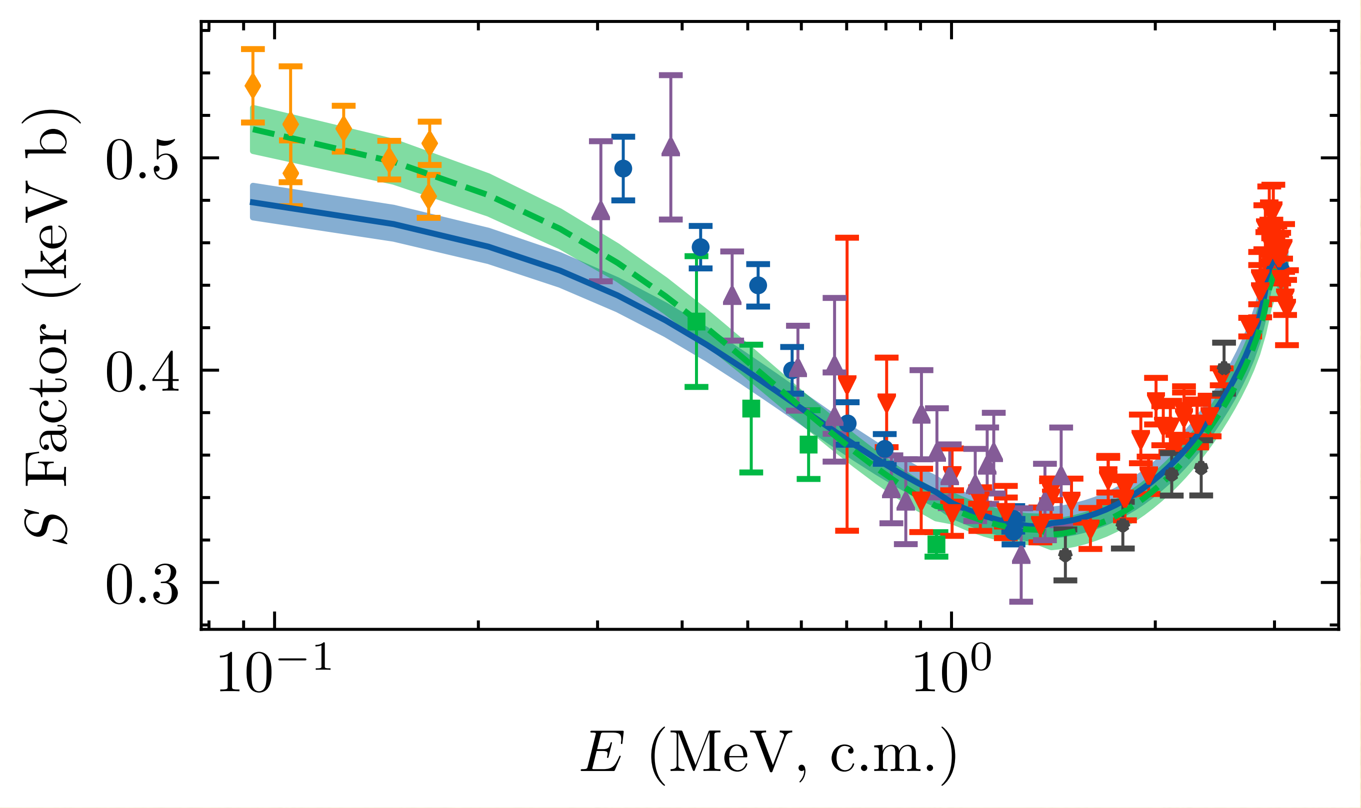

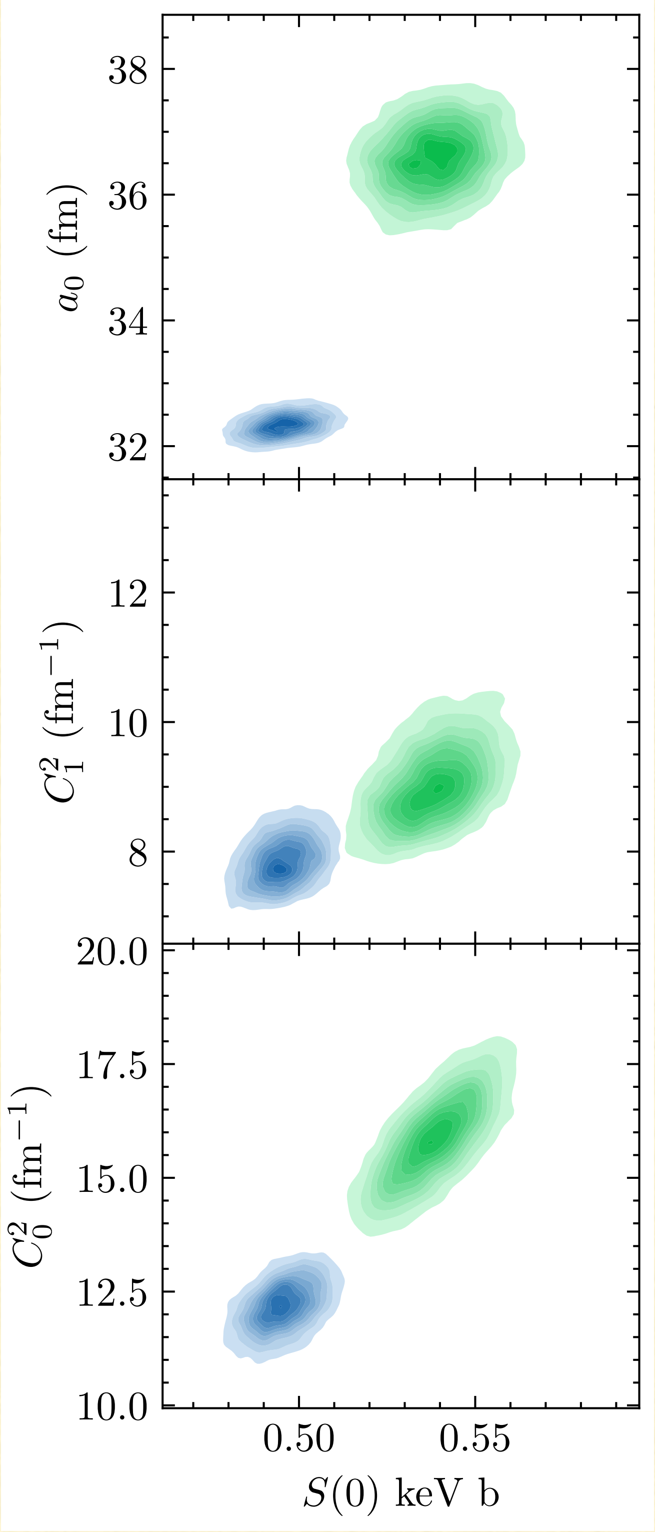

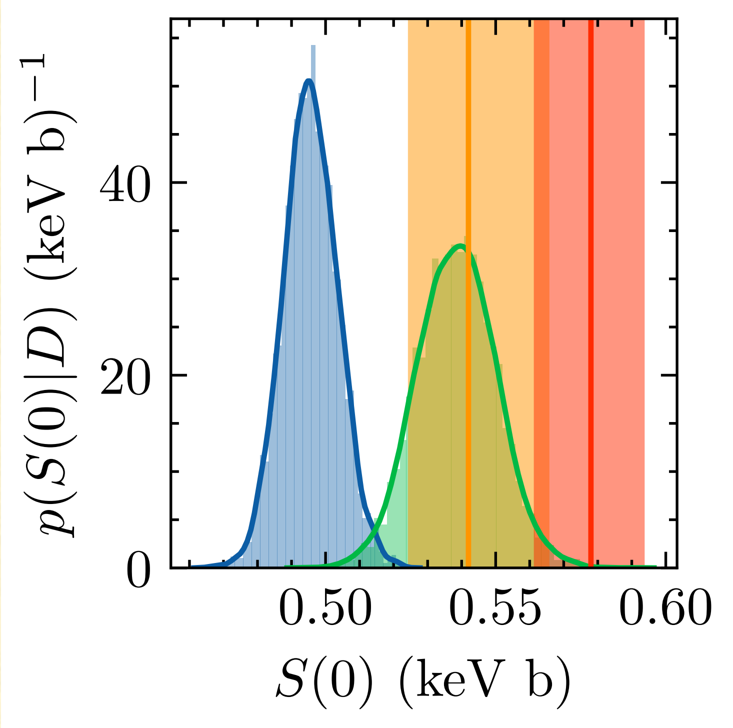

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Bayesian analysis of the dt reaction

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- Precise data for $E_{c.m}$=5-260 keV with stated normalization errors of 1.26-2.5%

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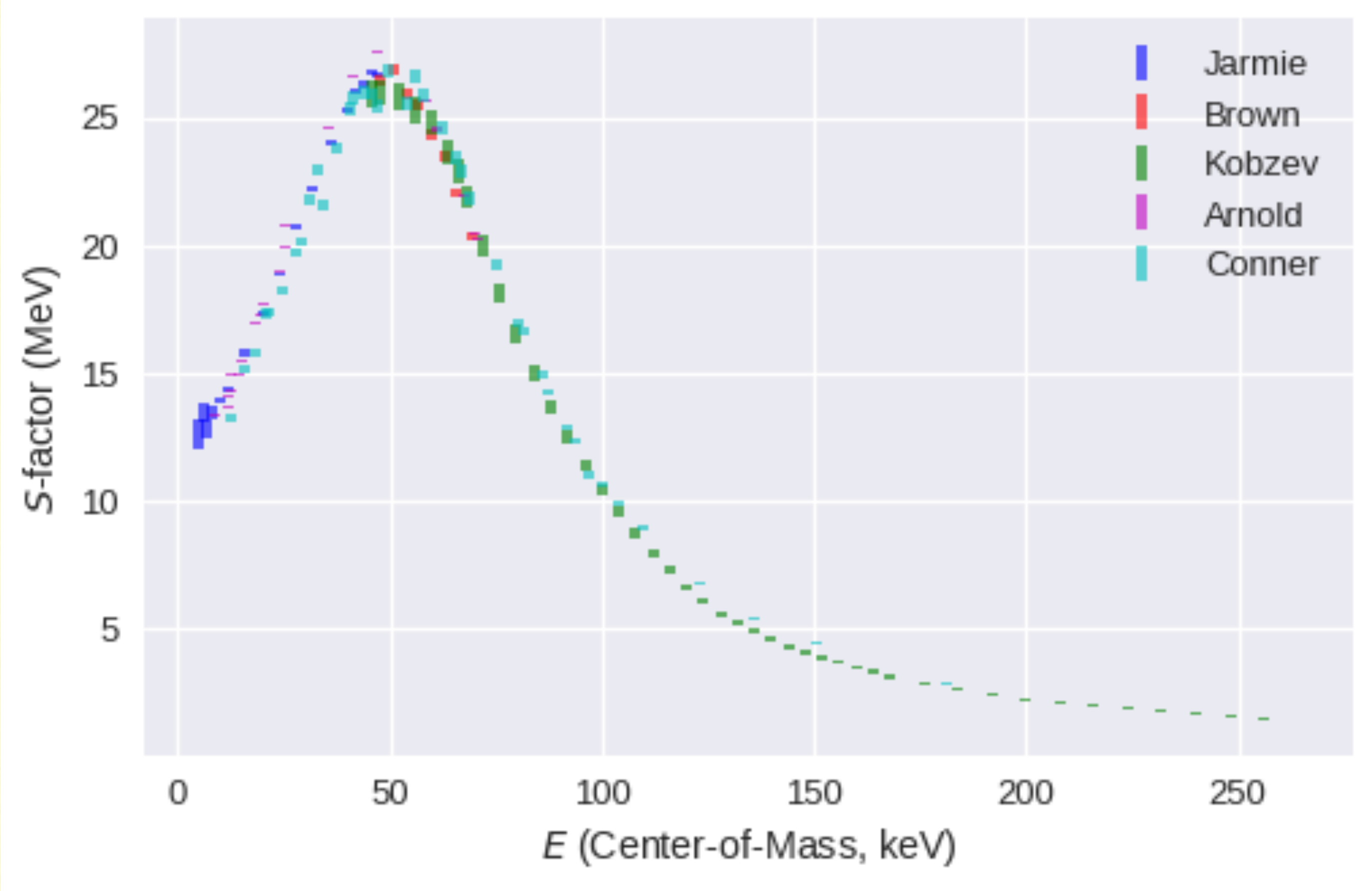

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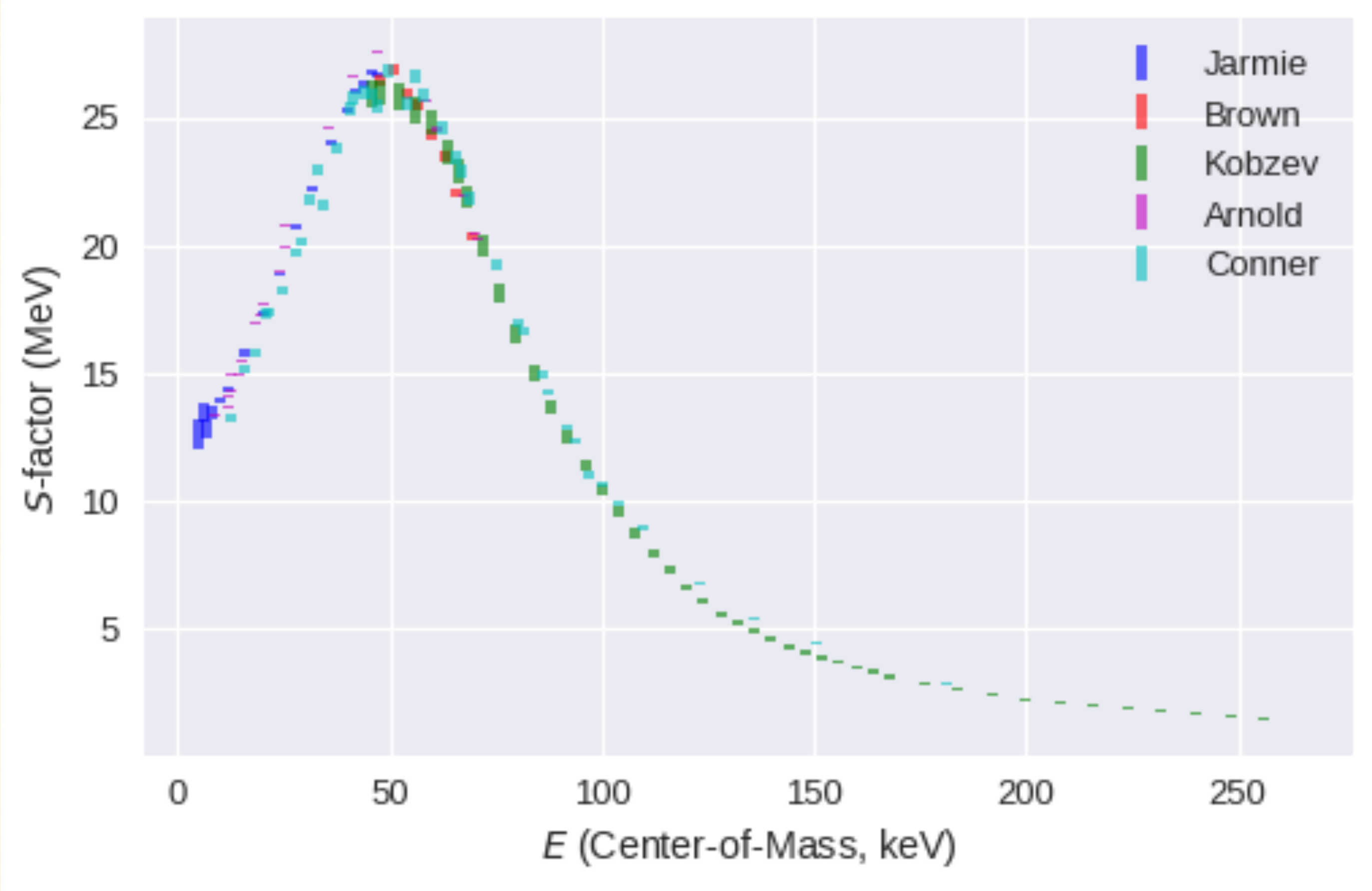
- Here we will use five data sets: Jarmie, Brown, Kobzev, Arnold, Conner
- Precise data for $E_{c.m}$=5-260 keV with stated normalization errors of 1.26-2.5%
- Goal: S(40 keV) plus error bar

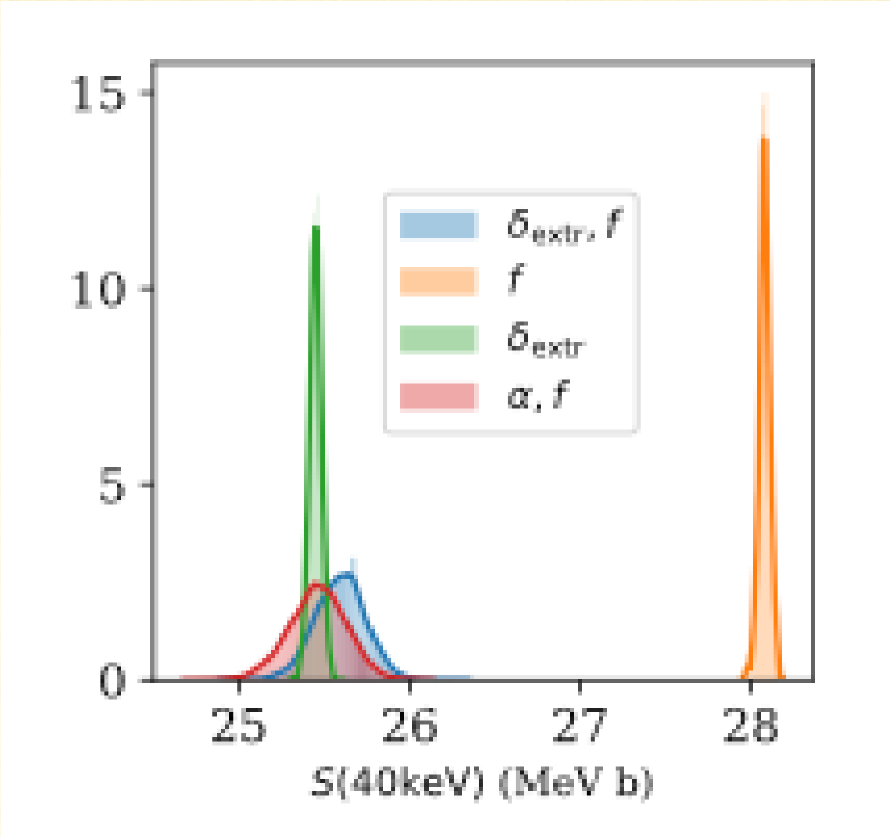


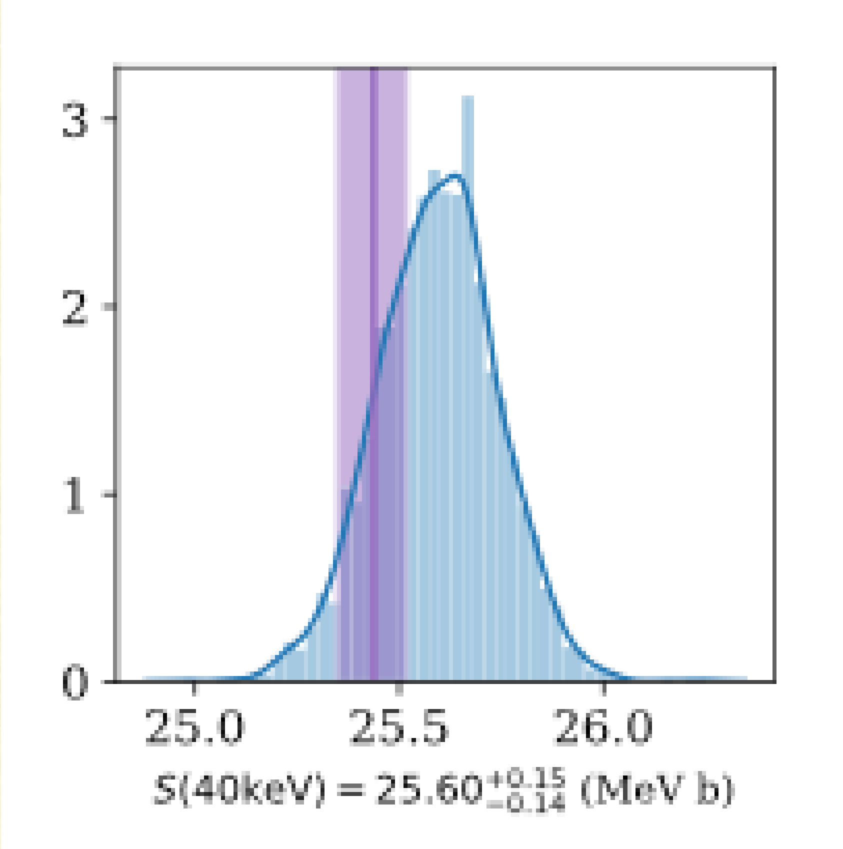
Improved statistical model

Odell, Brune, DP, Phys. Rev. C (2022) cf. de Souza et al., Phys. Rev. C (2019)

A. Include "extrinsic errors": additional point-to-point uncertainty, added in quadrature to nominal statistical error. Take $\sigma_{extr, j}$ to be one number in MeV.b for each data set j and sample it to infer what it might be.

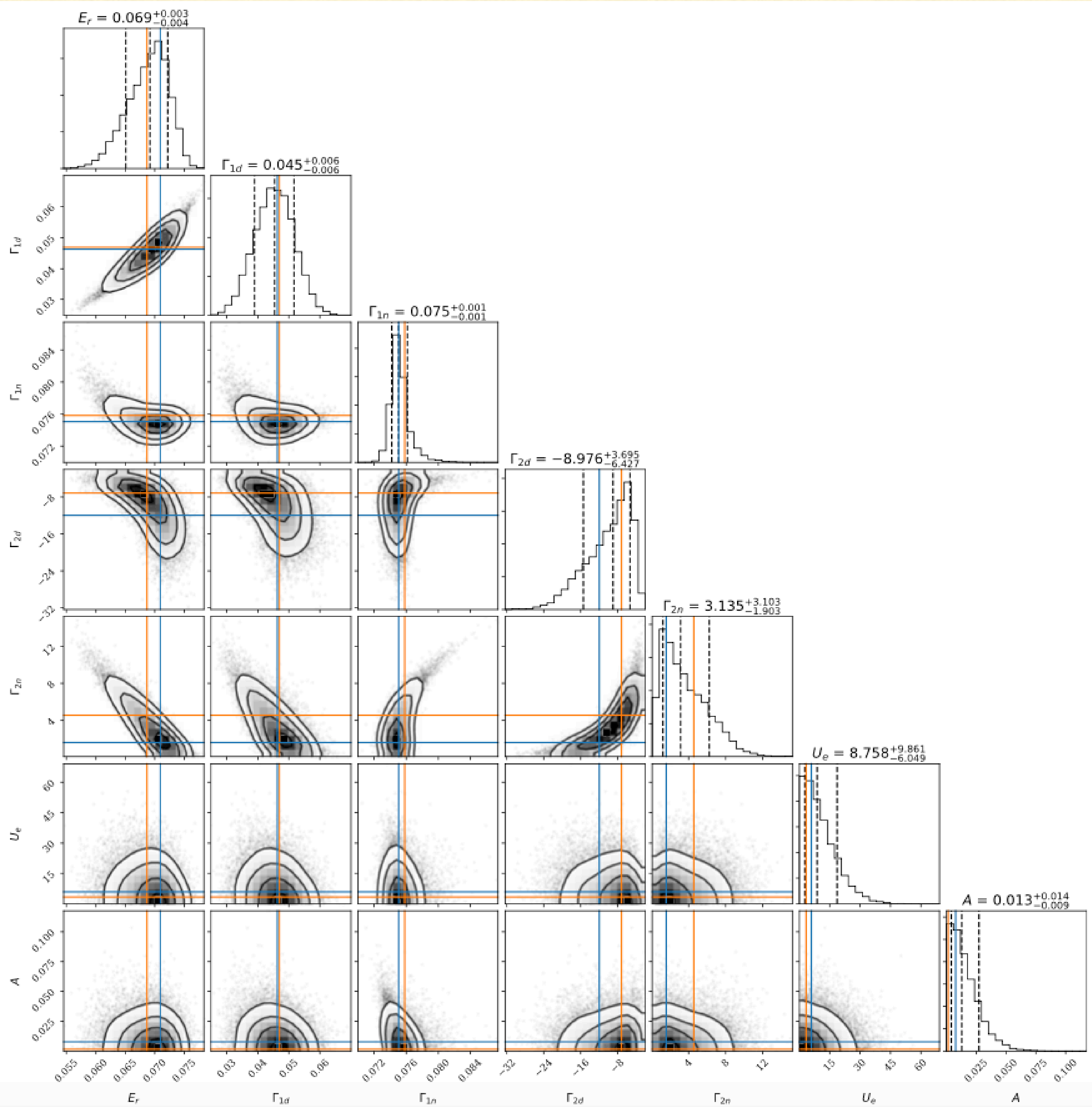
B. Take $\sigma_{\rm point-to-point} = \sqrt{\sigma_{i,j}^2 + \alpha_j^2 S_{i,j}^2}$ with α_j common to all points in data set j. (Relative extrinsic uncertainty rather than absolute extrinsic uncertainty.)





Purple:
de Souza et al.

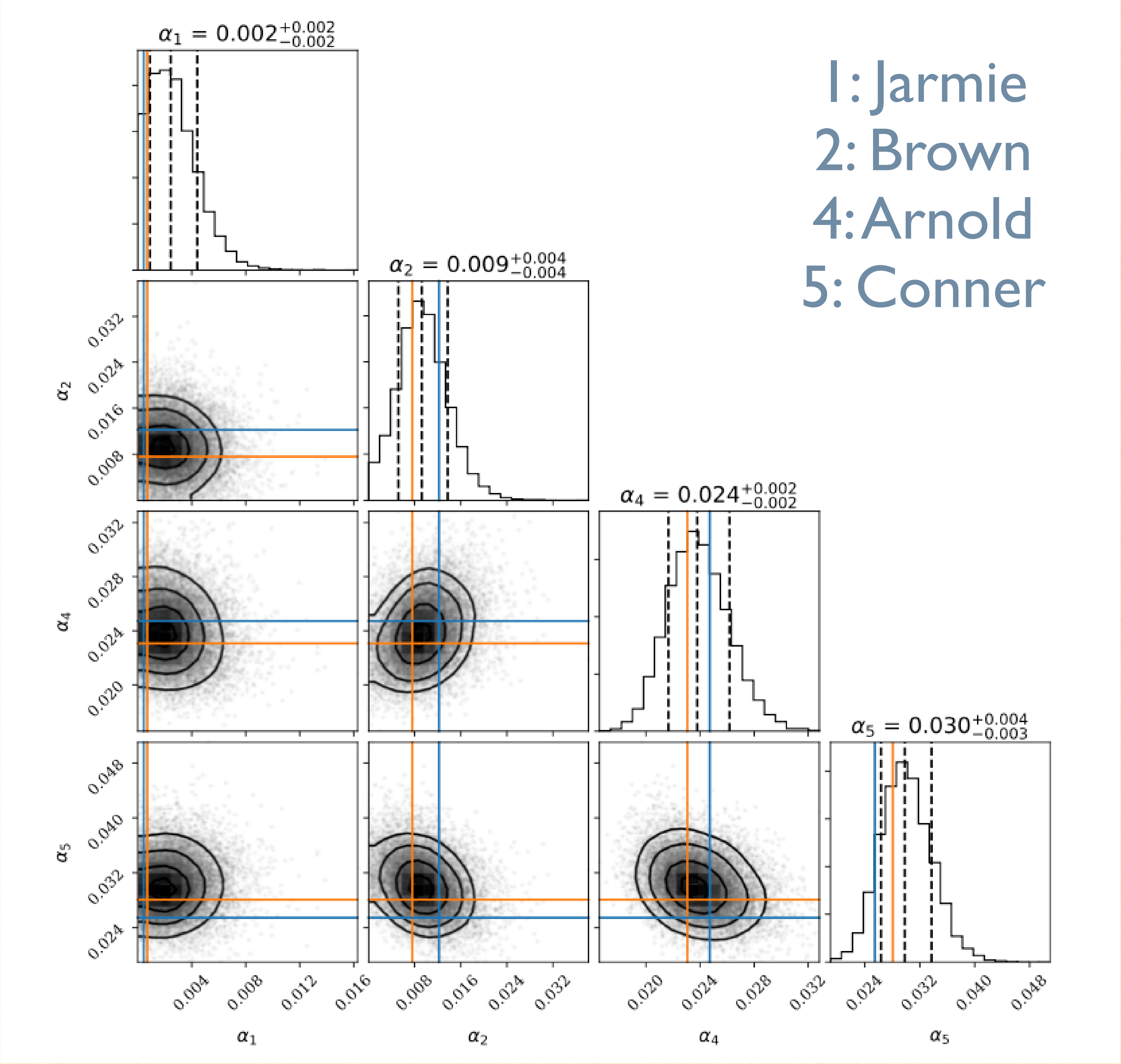
Posteriors for our best model



R-matrix parameters

- ^{5}He 3/2+ resonance energy
- ^{5}He 3/2+ resonance d width
- ^{5}He 3/2+ resonance n width
- ^{5}He 3/2+ background resonance parameters
- Screening potential
- ^{5}He 1/2+ background resonance parameter combination

Posteriors for our best model



R-matrix parameters

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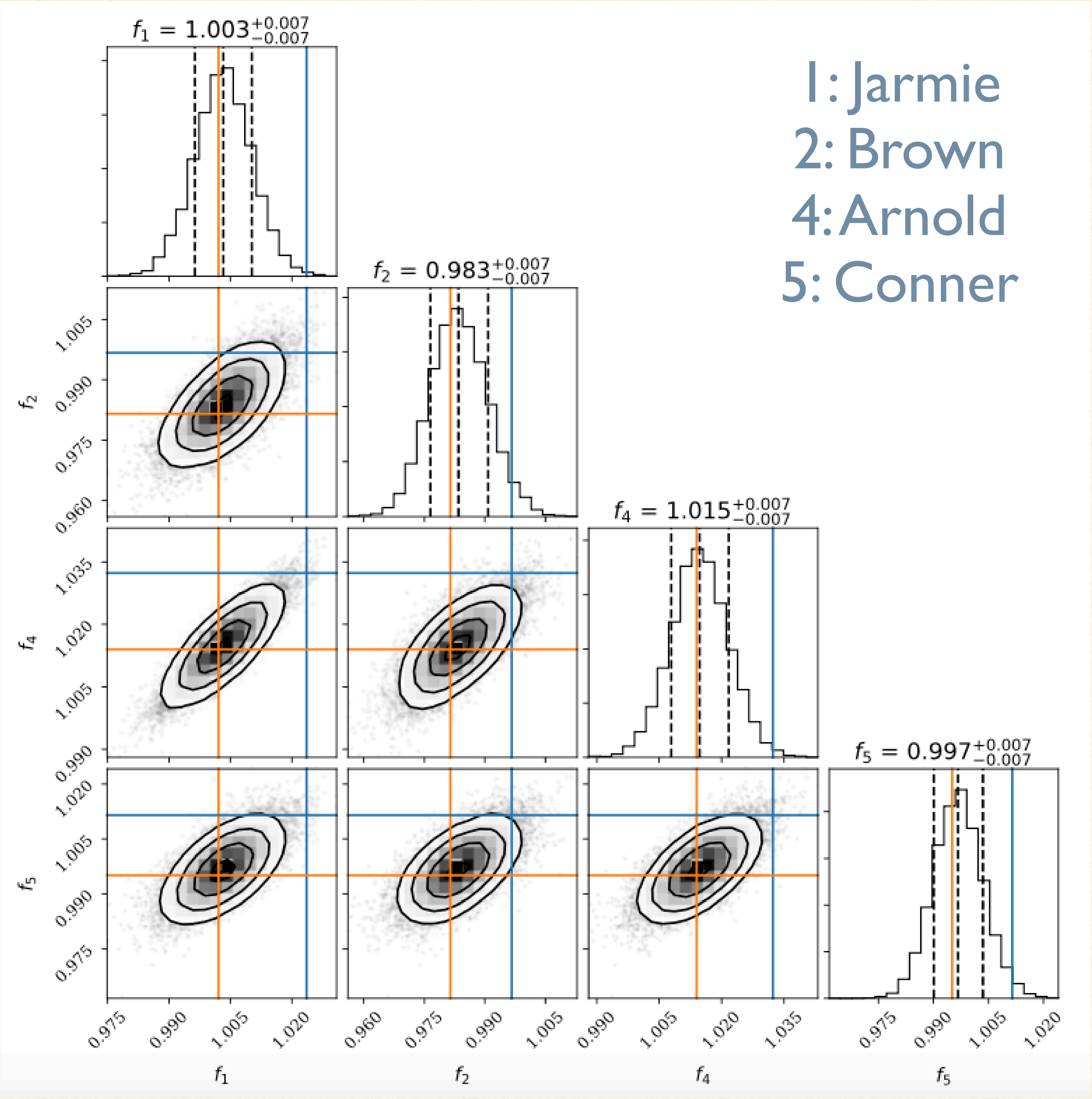
Relative extrinsic uncertainty and normalization for each data set

Posteriors for our best model



R-matrix parameters

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Relative extrinsic uncertainty and normalization for each data set

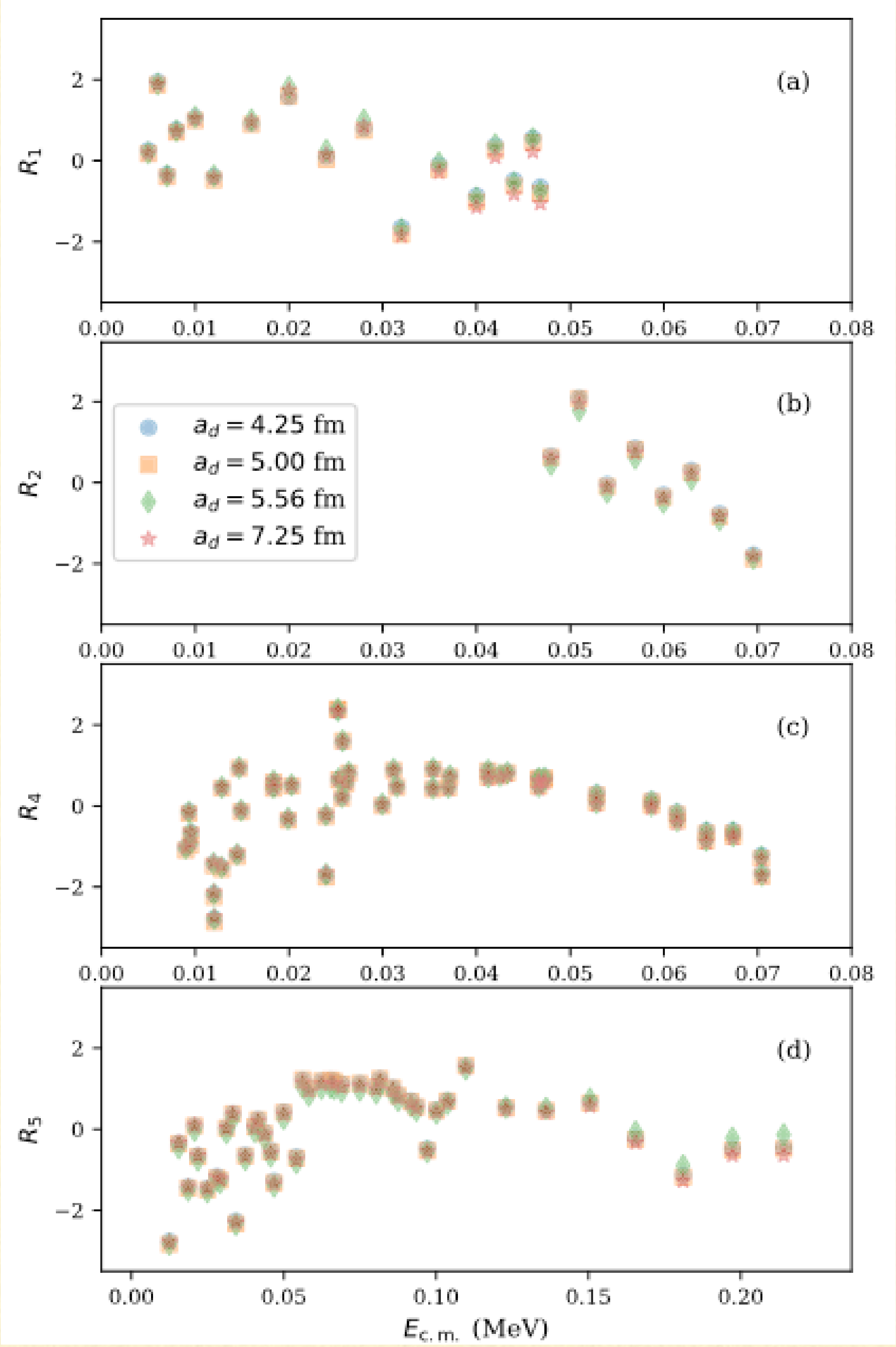
Residuals

Jarmie

Brown

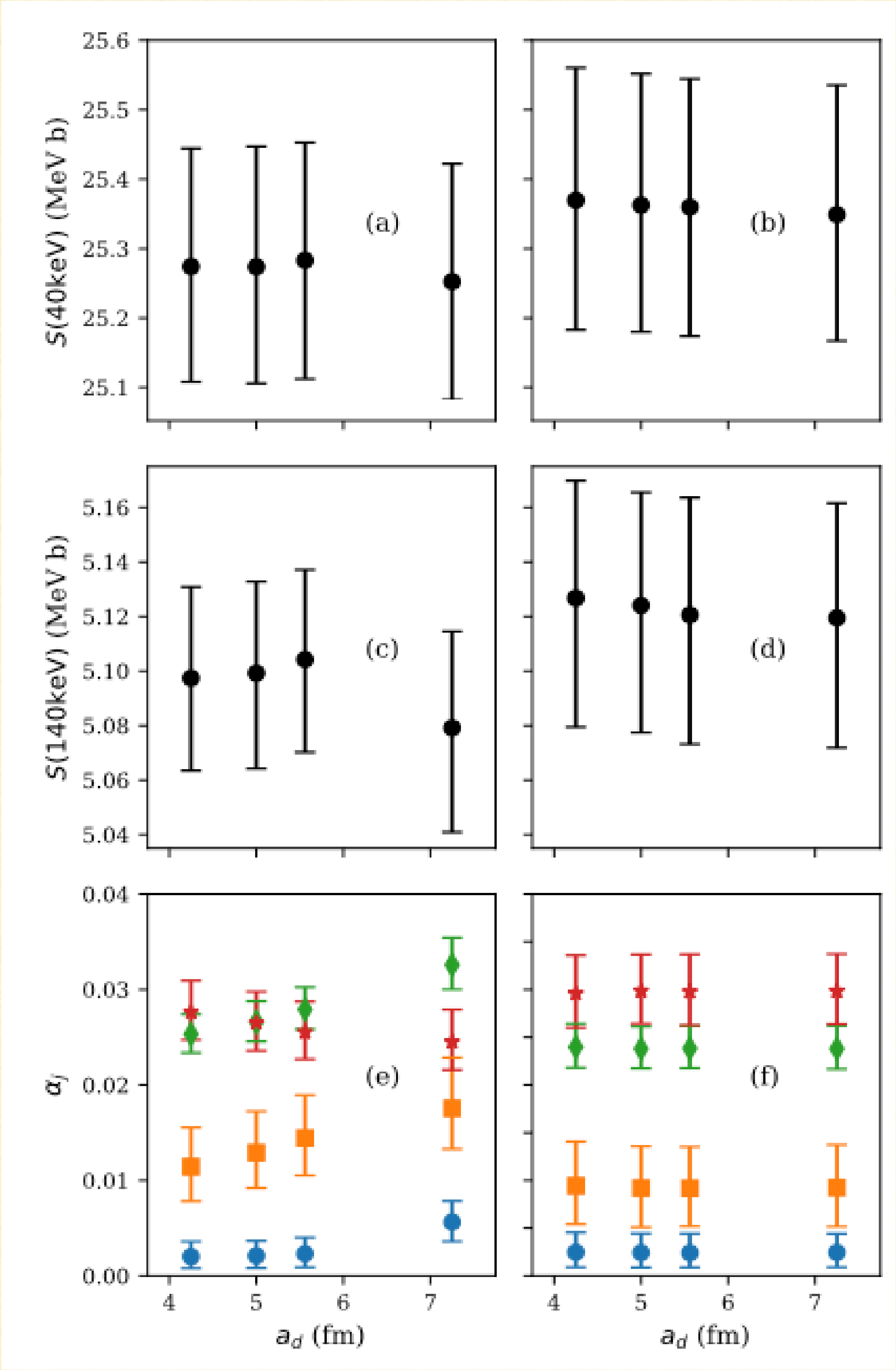
Arnold

Conner



cf. Kobzev residuals

Result, comparisons, implications



- Best R-matrix model also includes 1/2+ background level, and 3/2+ background level
- Physical results are then independent of channel radius
- Extrinsic errors needed for consistency, experimental norms. then more uncertain
- S(40 keV)=25.36 ± 0.19 MeV · b
- Consistent with de Souza et al., but with error bar that is roughly 2 x bigger
- cf. Bosch & Hale (1993): S(40 keV)=25.87 ± 0.49 MeV · b

Further applications of BRICK

- $^{19}F(p,\gamma)^{20}Ne$ – Zhang et al. (incl. deBoer, Odell) Nature **610**, 656-660 (2022)
    - Low-energy resonance opens up possibility of "warm" CNO breakout
- $^{10}B(p,\alpha)^{7}Be$ – Van de Kolk et al. (incl. deBoer, Odell) PRC **105**, 055802 (2022)
    - possible temperature probe for $^{11}B(p,2\alpha)^{4}He$ – aneutronic plasma fusion source
- $^{23}Na(p,\gamma)^{24}Mg$ – Boeltzig et al. (incl. deBoer, Odell) PRC **106**, 045801 (2022)
    - breakout reaction linking NeNa and MgAl cycles
- $^{13}C(\alpha,n_1)^{16}O$ – deBoer et al. (incl. deBoer, Odell) PRC **106**, 055808 (2022)
    - partial cross section measurement, improves BG modeling

Summary

- Parametric uncertainties in R-matrix analyses can be quantified by MCMC sampling of the Bayesian posterior and evaluating derived quantities
- https://github.com/odell/brick

Bayesian Analysis of Nuclear Dynamics

- Multiple examples of successful application to different reactions
- Enables more sophisticated modeling of experimental imperfections
- Knowledge of full posterior provides access to parameter correlations, allows diagnosis of which parameters are not needed, shows where there is multi-modality, non-Gaussianity, and more
- Error propagation to derived quantities is straightforward with samples in hand
- Model checking (residuals, coverage, etc.) needs to be done at end
- Model uncertainties of R-matrix analysis? Comparison to EFT, ab initio, etc.