Light Element Covariances

from LANL-EDA R-matrix analyses

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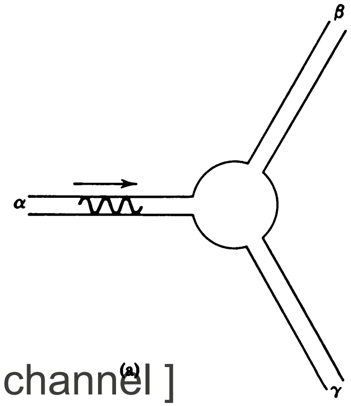
Outline

- **Formalism**
  - Multipartite, multichannel, unitary R-matrix approach
- **Uncertainty quantification**
  - parameter uncertainty
  - observable covariance
- **New/updated evaluations with covariance information**
  - `n-001_H_001`
  - `n-003_Li_006`
  - `n-005_B_010`
  - `n-006_C_012`
  - `n-008_O_016`

R-matrix formalism/LANL-EDA code



- **À la Wigner & Eisenbud**
  - Multipartite [*e.g.* ^{7}Li (t+^{4}He, n+^{6}Li, …)]
  - Multichannel [J^{π} = L+S, …, |L-S|]
  - Ensures unitarity [essential for correct normalizations]
- **Parametrization form**
  - R-matrix parameters: pole positions, residues [per partition & channel]
  - Relativistic [important for narrow resonances, esp. near-threshold]
- **Observables**
  - Partition type
    - 2➔2 only
    - spectra 2➔3, 2➔4, etc handled by auxiliary code
    - particle channels [n, p, D, T, ^{3}He, α, ...]
    - electromagnetic [*e.g*. p(n,γ)d]
  - Any/all polarization/unpolarized observables
    - total, angle-integrated, angular distribution, excitation functions, single-spin asymmetries, spin rotations, spin correlation functions, …
- **Fit quality**
  - typical χ^2/dof ~ 1.2 – 1.5

Uncertainties from chi-squared minimization

$$\chi^2_{\rm EDA} = \sum_i \left[\frac{nX_i(\mathbf{p}) - R_i}{\Delta R_i}\right]^2 + \left[\frac{nS-1}{\Delta S / S}\right]^2$$

$$\begin{cases} R_i,\ \Delta R_i = \text{relative measurement, uncertainty} \\ S,\ \Delta S = \text{experimental scale, uncertainty} \\ X_i(\mathbf{p}) = \text{observable calc. from res. pars. } \mathbf{p} \\ n = \text{normalization parameter} \end{cases}$$

Near a minimum of the chi-squared function at $\mathbf{p} = \mathbf{p}_0$:

$$\chi^2(\mathbf{p}) = \chi^2_0 + (\mathbf{p}-\mathbf{p}_0)^{\rm T}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\rm T}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0)$$
$$= \chi^2_0 + \Delta\chi^2.$$

$$\begin{cases} \chi^2_0 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

Conventions:

1) previous: $\Delta\chi^2 = 1 \implies$ Very small uncertainties $\delta p_i = (C^0_{ii})^{1/2} \sim \mathcal{O}(N_p^{-1/2})$

2) improved: $\Delta\chi^2 = \tfrac{1}{2}\Delta\mathbf{p}^{\rm T}\mathbf{G}_0\Delta\mathbf{p} \le \Delta\chi^2_{\max}$,

$$P(\Delta\chi^2 | k) = \left[2^{\frac{k}{2}}\Gamma(\tfrac{k}{2})\right]^{-1}\int_0^{\Delta\chi^2_{\max}} t^{\frac{k}{2}-1}e^{-\frac{t}{2}}dt = \text{CL (e.g.} \sim 0.68 \text{ for 1-}\sigma\text{), 0.95 for 2-}\sigma\text{, etc.}$$

$$\Delta\chi^2_{\max} \approx k = \langle \Delta\chi^2 \rangle.$$

$$\delta p_i \sim (N_p C^0_{ii})^{1/2}$$

Covariance

The parameter covariance matrix is $\mathbf{C}_0 = 2\mathbf{G}_0^{-1}$, and so first-order error propagation gives for the cross-section covariances

$$\chi^2(\mathbf{p}) = \chi_0^2 + (\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0) \quad \begin{cases} \chi_0^2 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

$$= \chi_0^2 + \Delta\chi^2.$$

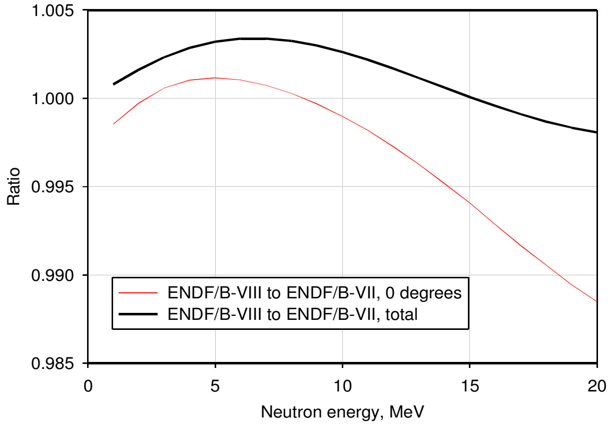
$$\mathrm{cov}[\sigma_{\mathrm{i}}(E)\sigma_j(E')] = \left[\nabla_{\mathbf{p}}\sigma_{\mathrm{i}}(E)\right]^{\mathrm{T}}\mathbf{C}_0\left[\nabla_{\mathbf{p}}\sigma_{\mathrm{j}}(E')\right]\Big|_{\mathbf{p}=\mathbf{p}_0}$$

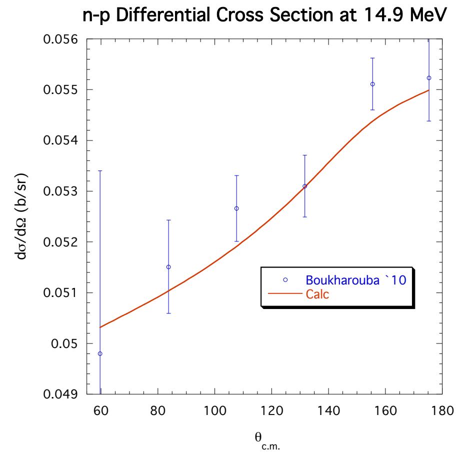
$$= \Delta\sigma_{\mathrm{i}}(E)\Delta\sigma_{\mathrm{j}}(E')\rho_{ij}(E,E').$$

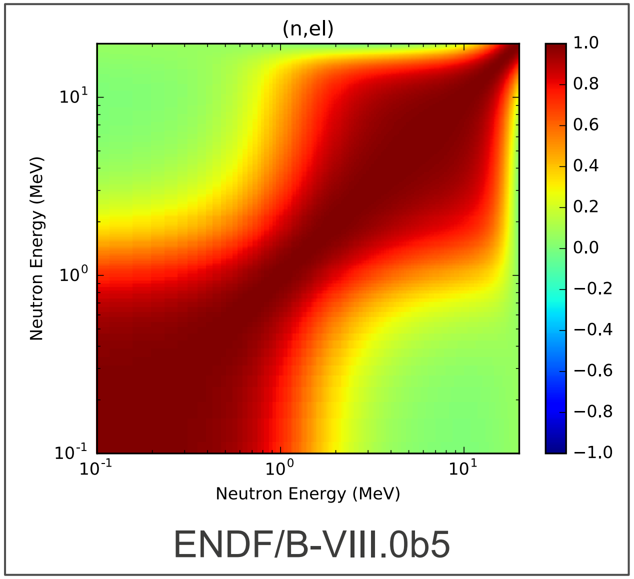
observable uncertainties

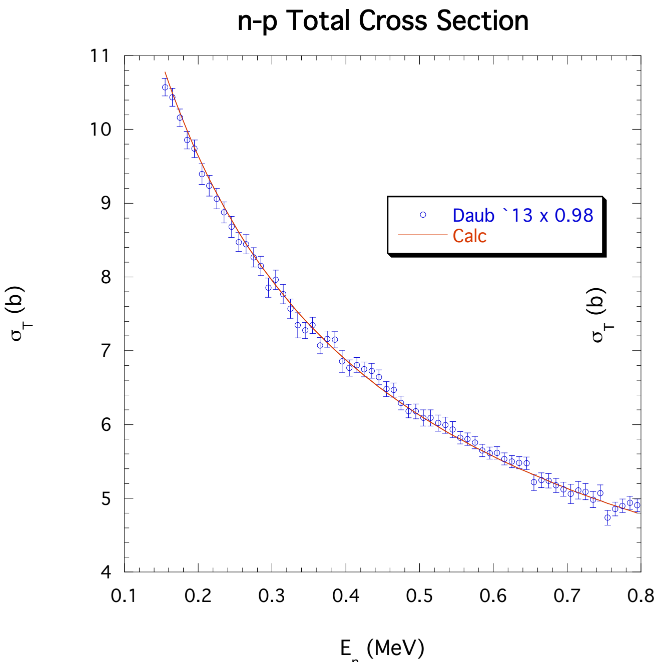
correlation coefficient

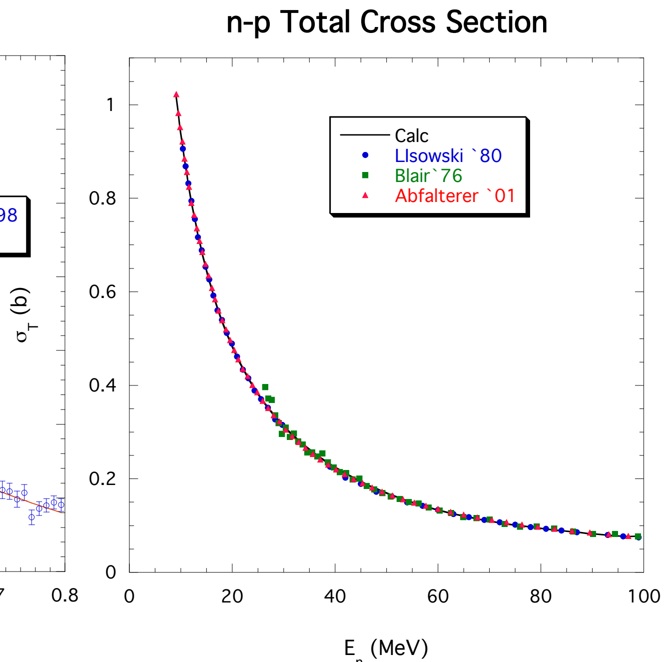
Evaluation 1: `n-001_H_001`











Partitions:

$$pp(\ell \leq 3); np(\ell \leq 3);$$
$$\gamma d(\ell \leq 1); nn(\ell \leq 3)$$

36 channels $(J^{\pi} LS)$

$$\chi^2/\text{dof} \simeq 0.9$$

Evaluation 2: `n-003_Li_006`

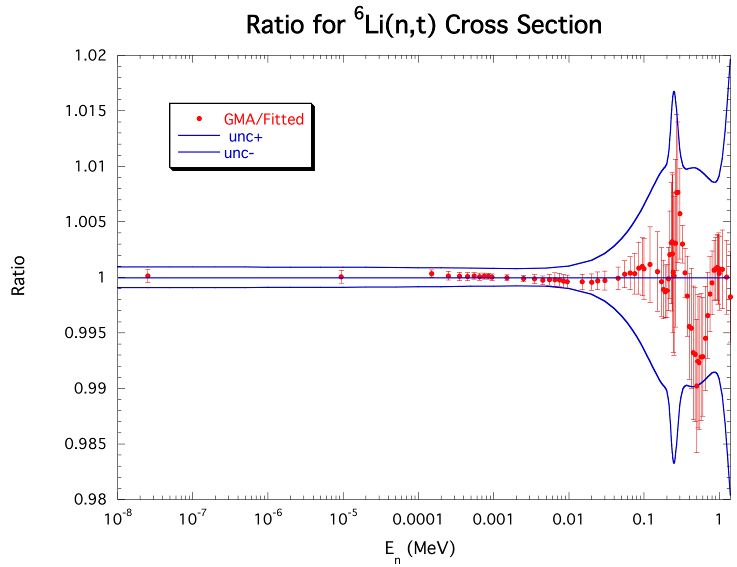
Partitions :

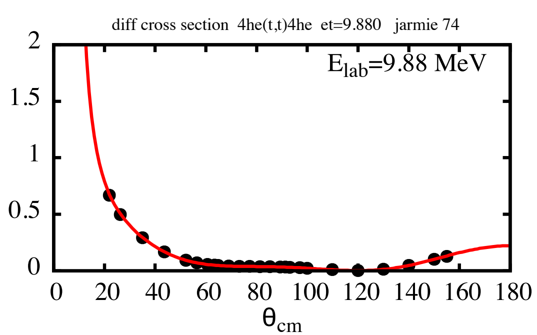
$t^4\mathrm{He}(\ell \leq 5); n^6\mathrm{Li}(\ell \leq 3);$

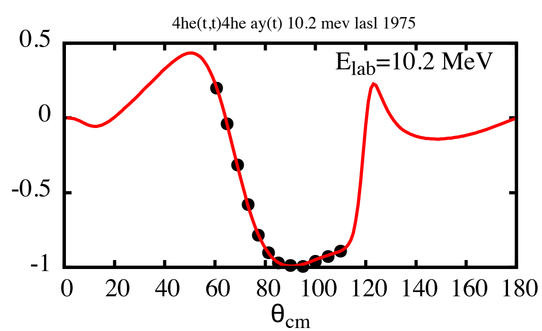
$n^6\mathrm{Li}^*(\ell \leq 1); d^5\mathrm{He}(\ell = 0)$

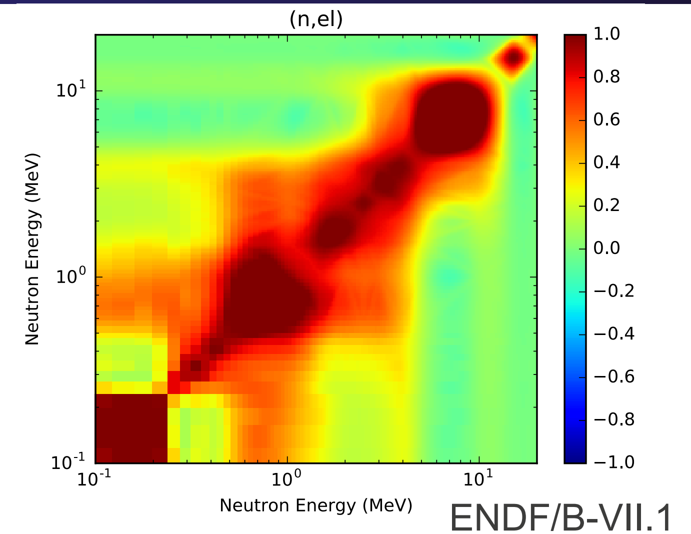
41 channels $(J^\pi LS)$

$\chi^2/\mathrm{dof} = 1.36$

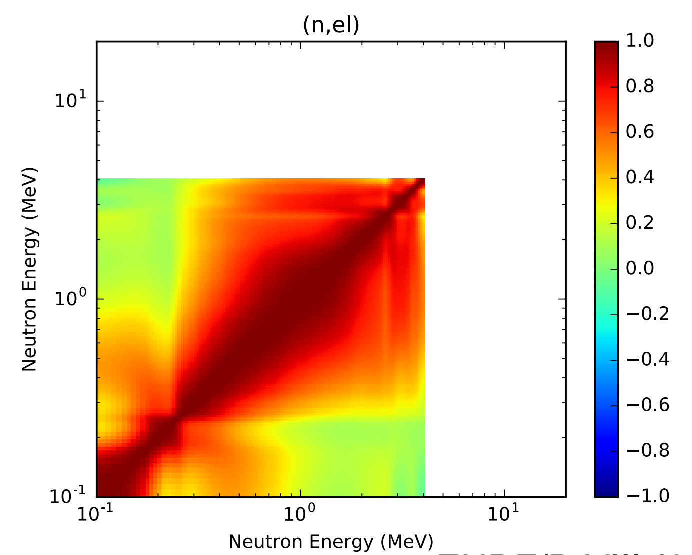








ENDF/B-VII.1



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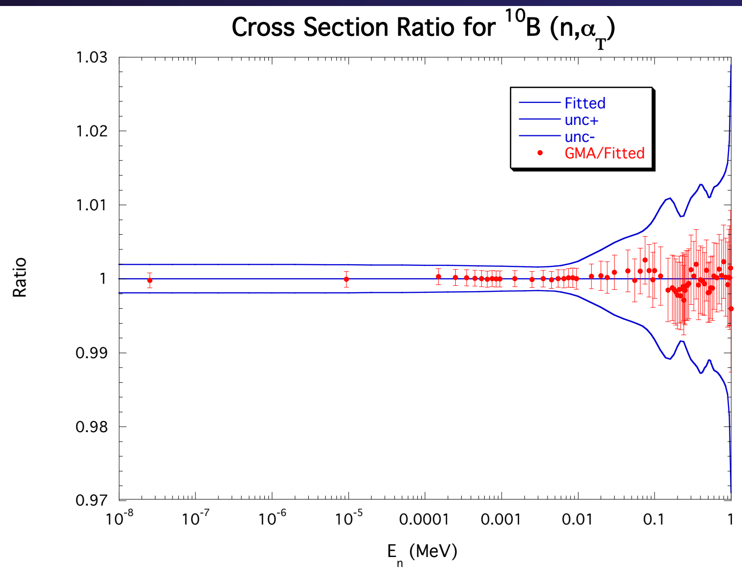
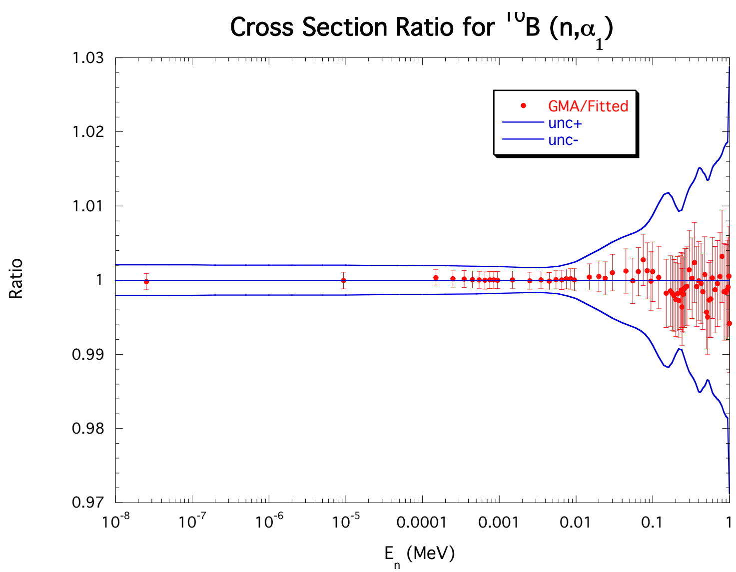
Evaluation 3: n-005_B_010





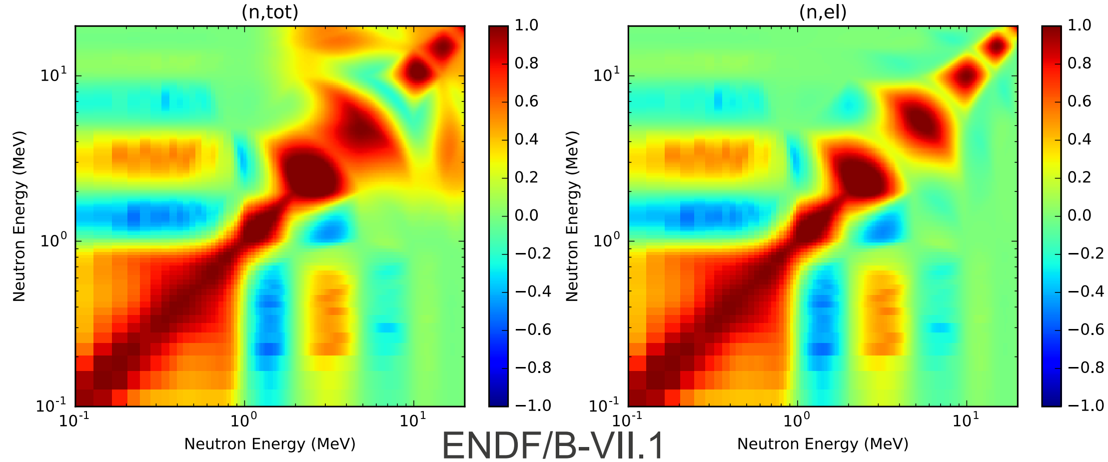
Partitions :

$n^{10}\mathrm{B}(\ell \leq 1); \alpha^{7}\mathrm{Li}(\ell \leq 3);$

$\alpha^{7}\mathrm{Li}^{*}(\ell \leq 1); t^{8}\mathrm{Be}(\ell \leq 2)$

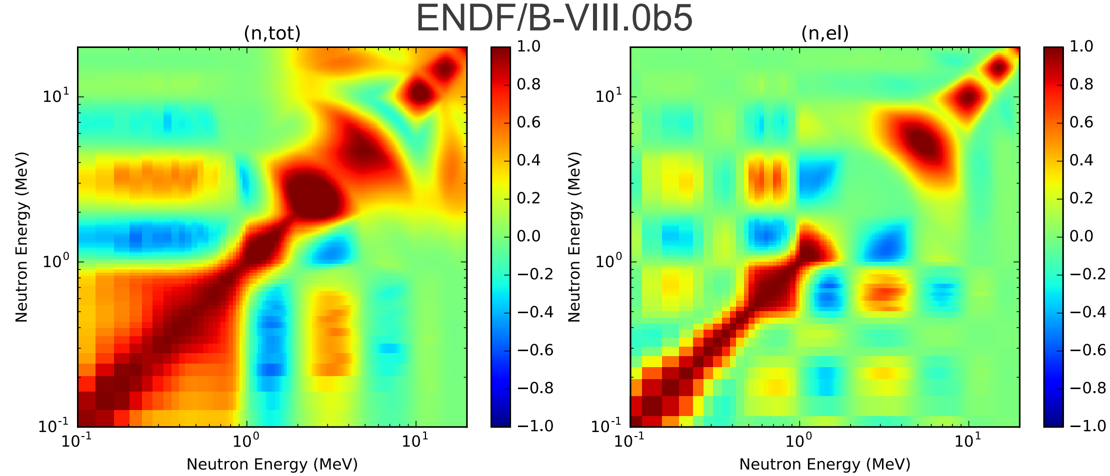
32 channels $(J^{\pi} LS)$

$\chi^2/\mathrm{dof} = 1.14$

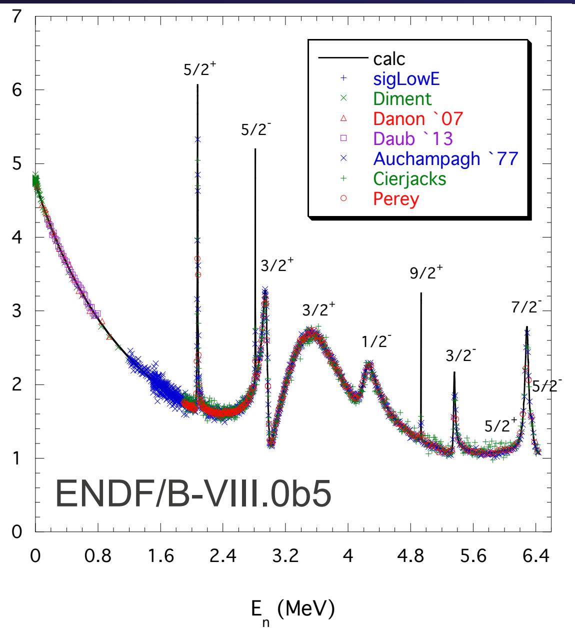


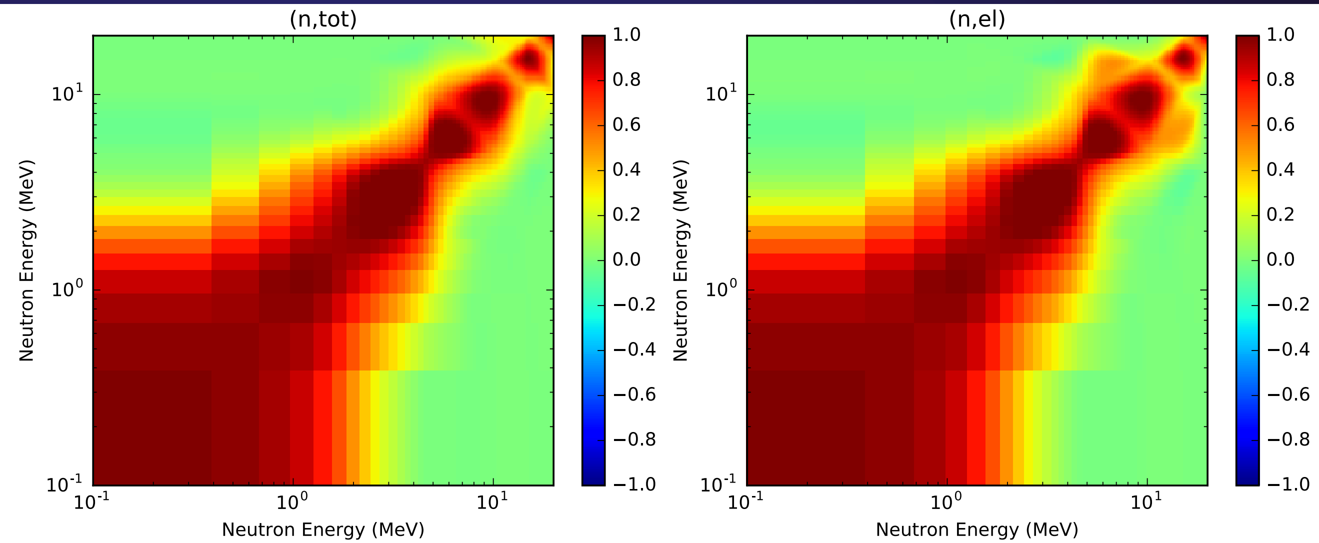
ENDF/B-VII.1

ENDF/B-VIII.0b5



Evaluation 4: `n-006_C_012`





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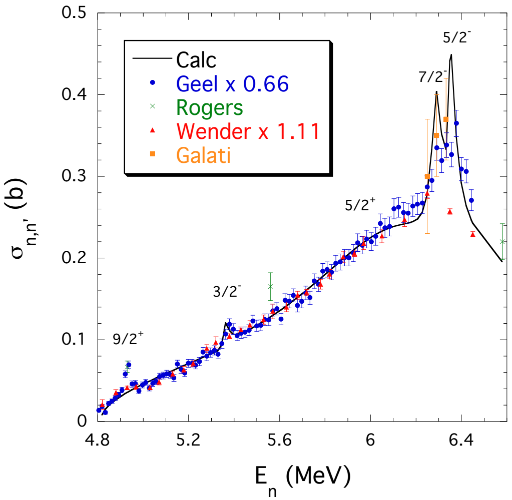
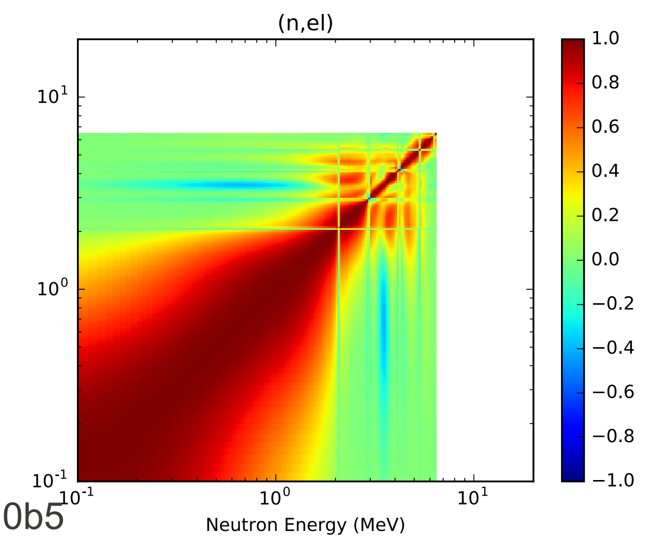


channel	a_c (fm)	l_{max}
n+^{12}C(0$^+$)	4.6	4
n+^{12}C*(2$^+$)	5.0	1
γ+^{13}C	50	1

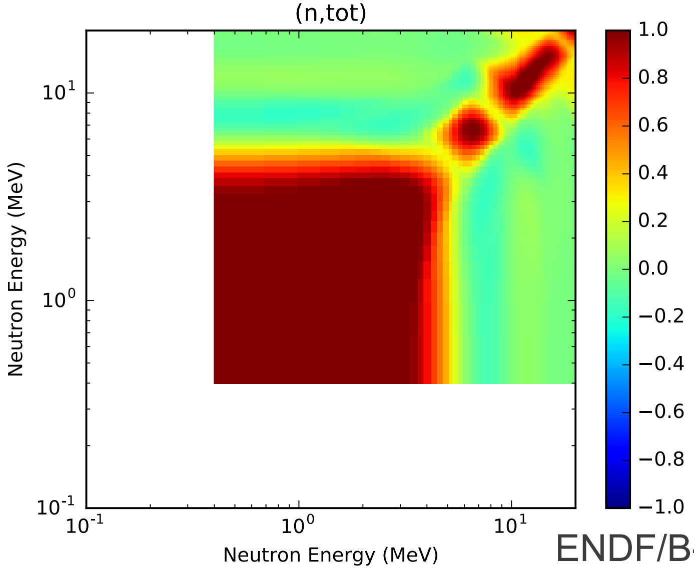
Reaction	Energies (MeV)	# data points	Data types
^{12}C(n,n)^{12}C	E_n = 0 – 6.45	6940	σ_T, $\sigma(\theta)$, $A_n(\theta)$
^{12}C(n,n')^{12}C*	E_n = 5.3 – 6.45	443	σ_{int}, $\sigma(\theta)$
^{12}C(n,γ)^{13}C	E_n = 0 – 0.199	7	σ_{int}
total	4994	7390	5

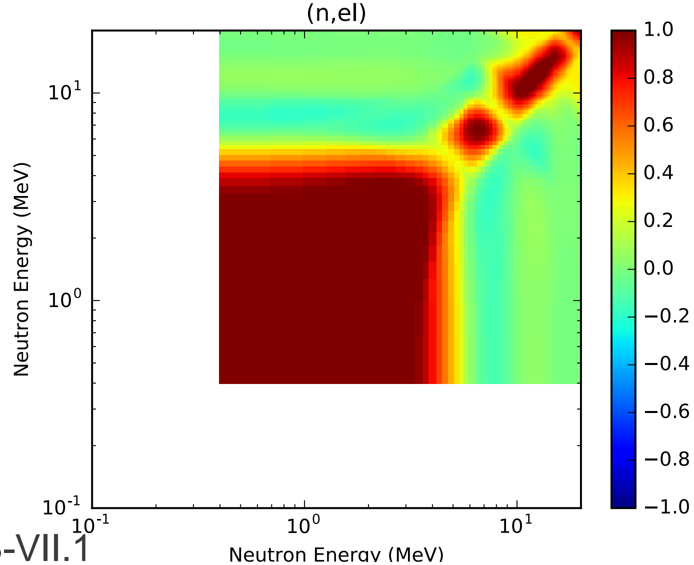
χ^2 per degree of freedom = 1.54



ENDF/B-VIII.0b5

Evaluation 5: n-008_O_016

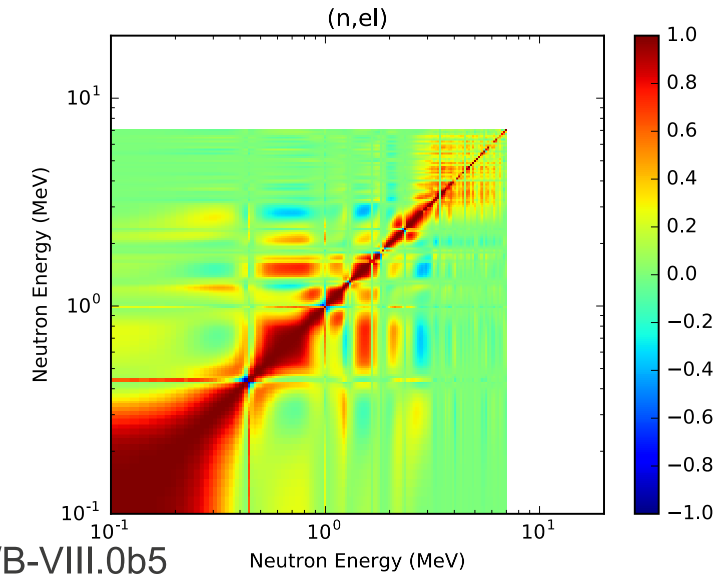




ENDF/B-VII.1

channel	a_c (fm)	l_{max}
n+^{16}O	4.4	4
α+^{13}C	5.4	5

Reaction	Energies (MeV)	# data points	Data types
^{16}O(n,n)^{16}O	E_n = 0 – 7	2540	σ_T, $\sigma(\theta)$, $P_n(\theta)$
^{16}O(n,α)^{13}C	E_n = 2.35 – 5	672	σ_{int}, $\sigma(\theta)$, $A_n(\theta)$
^{13}C(α,n)^{16}O	E_α = 0 – 5.4	870	σ_{int}
^{13}C(α,α)^{13}C	E_α = 2 – 5.7	1168	$\sigma(\theta)$
total		5250	8



χ^2 per degree of freedom = 1.68

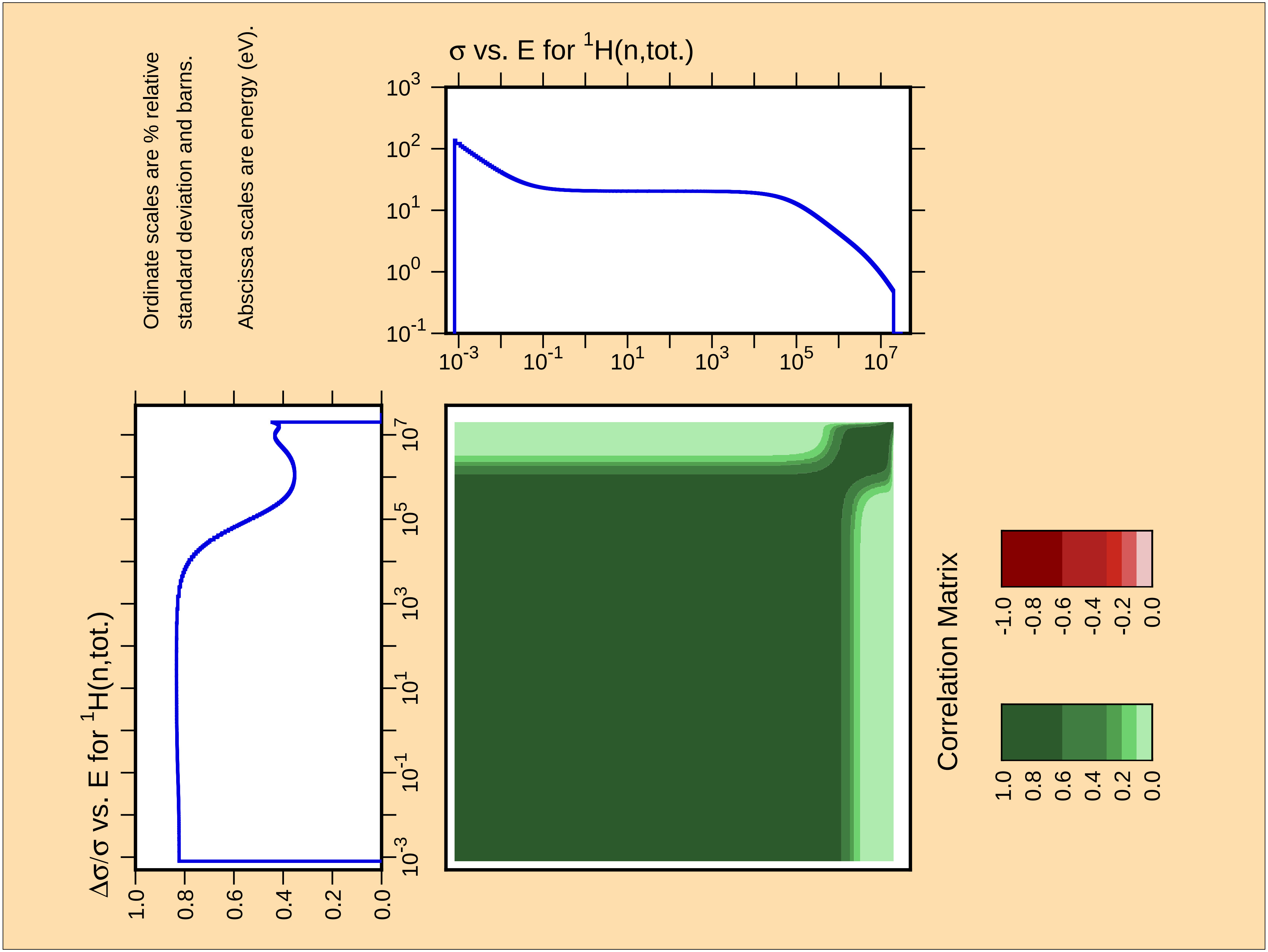
ENDF/B-VIII.0b5

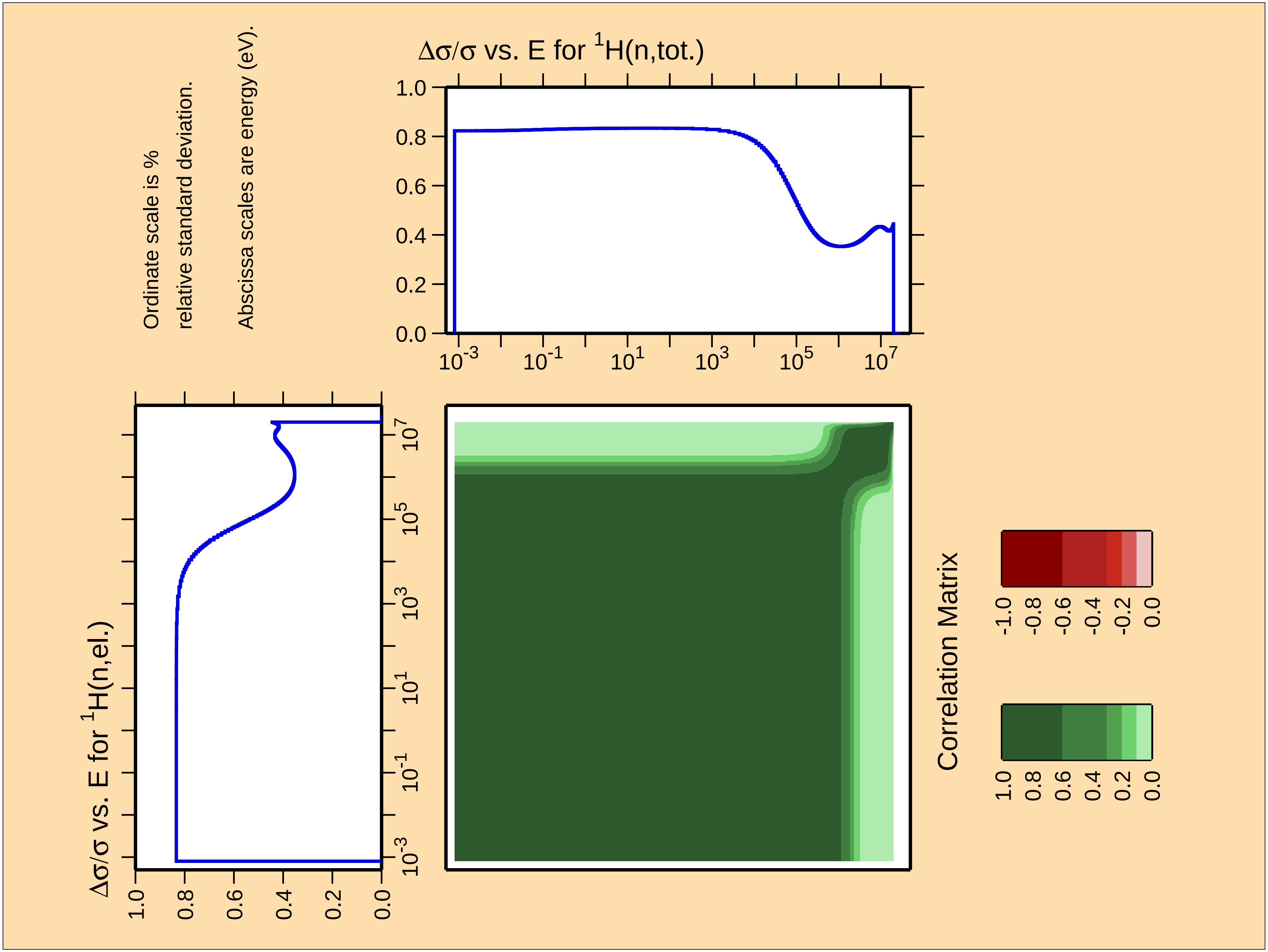
Outlook

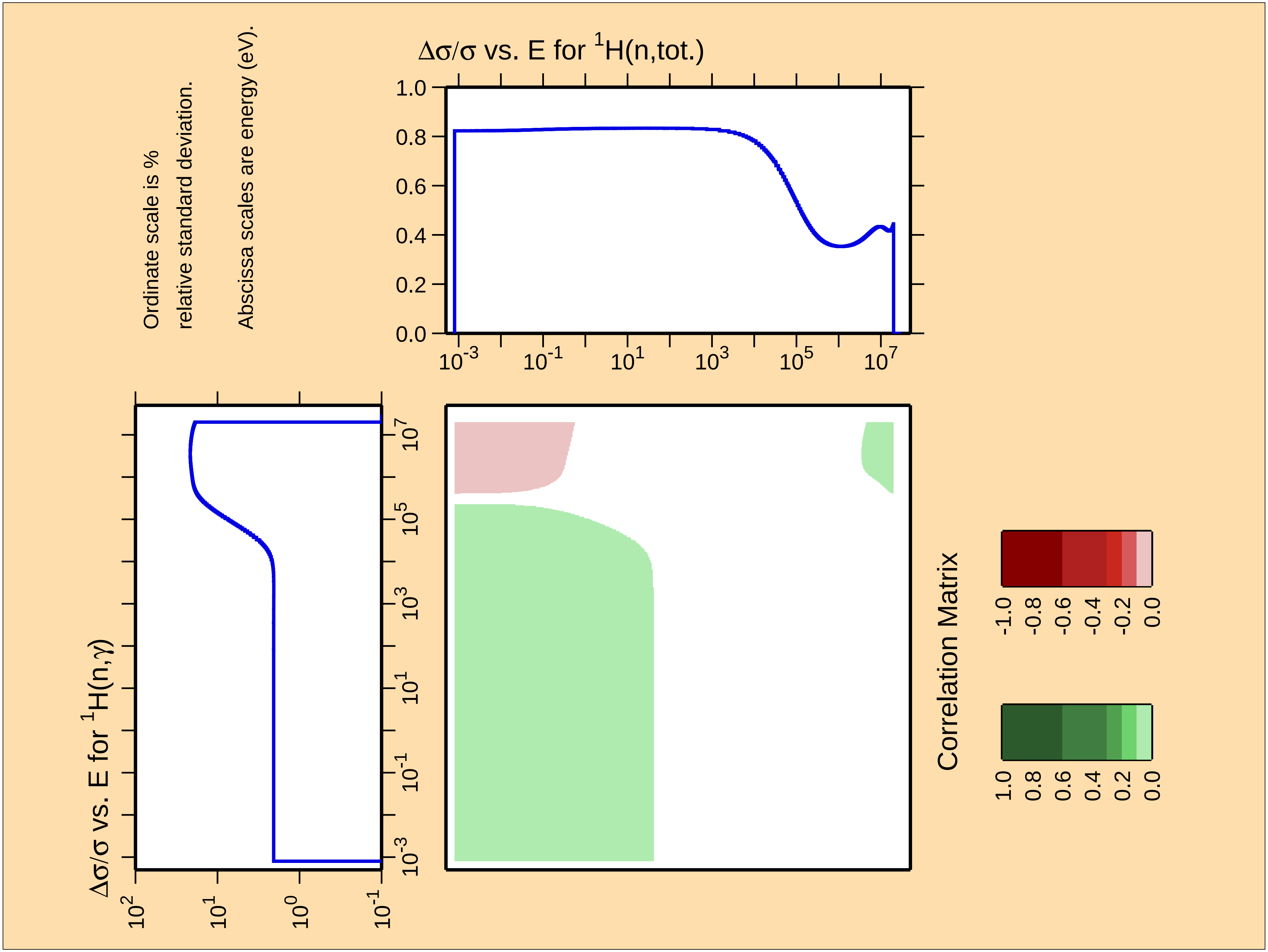
- **Short term**
  - – publish existing evaluations (including, of course, charged-particle) absent from ENDF/B
    - including all R-matrix & normalization parameters (Ian T.'s talk)
    - *Caveat Emptor*: EDA5 & 6 – relativistic parametrization
  - – use existing EDA5
- **Medium term**
  - – continue development on EDA6 (modern-language successor to EDA5)
    - primary objectives:
      - – extend light-element analyses/covariance to $E_n \leq 20$ MeV
      - – charged particles
      - – spectra
  - – Likelihood-based fitting with Bayesian approach
- **Long term**
  - – modern-language modular/OO structure will allow
    - experimental acceptance, efficiency, general IRF capabilities (comparable to SAMMY)
    - integrated, ***homogeneous*** optimization with integral benchmarks & other evaluation codes
      - – avoids 'optimization via email' situation that currently obtains

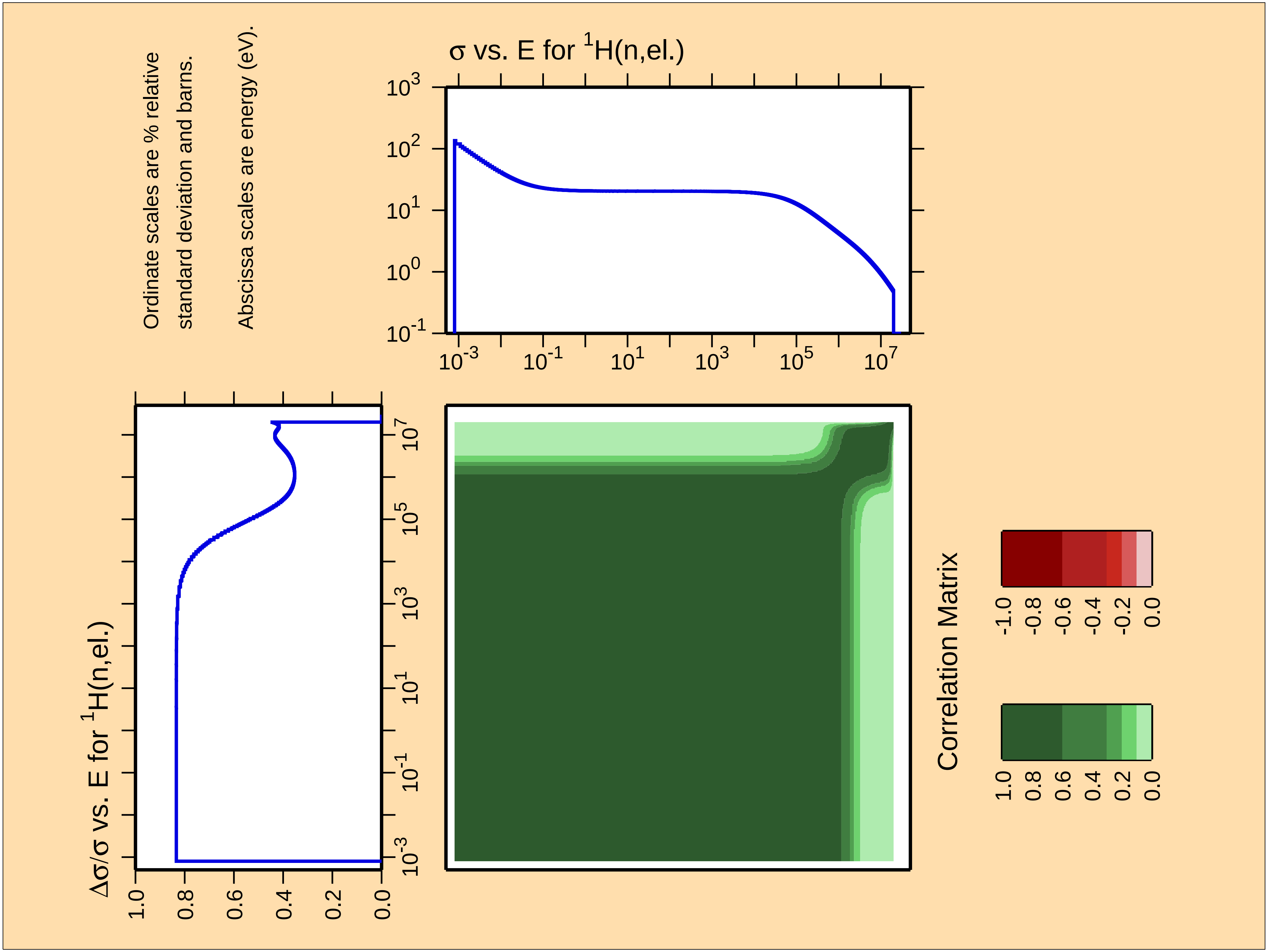
Thank you!

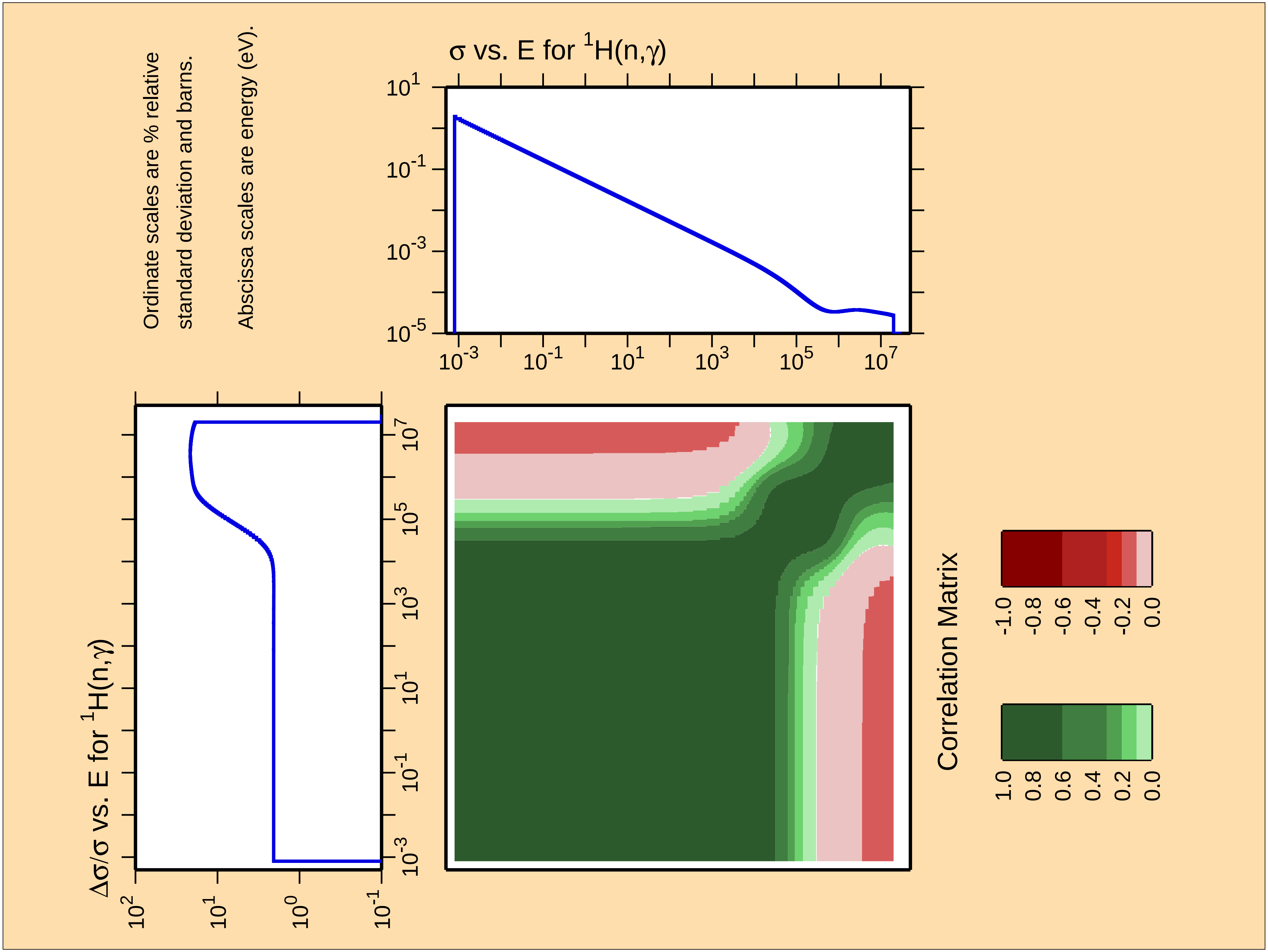
NJOY covariance output
courtesy of D. Brown


σ vs. E for 1H(n,tot.)
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
Δσ/σ vs. E for 1H(n,tot.)
Correlation Matrix
10^3
10^2
10^1
10^0
10^-1
10^-3
10^-1
10^1
10^3
10^5
10^7
1.0
0.8
0.6
0.4
0.2
0.0
-1.0
-0.8
-0.6
-0.4
-0.2

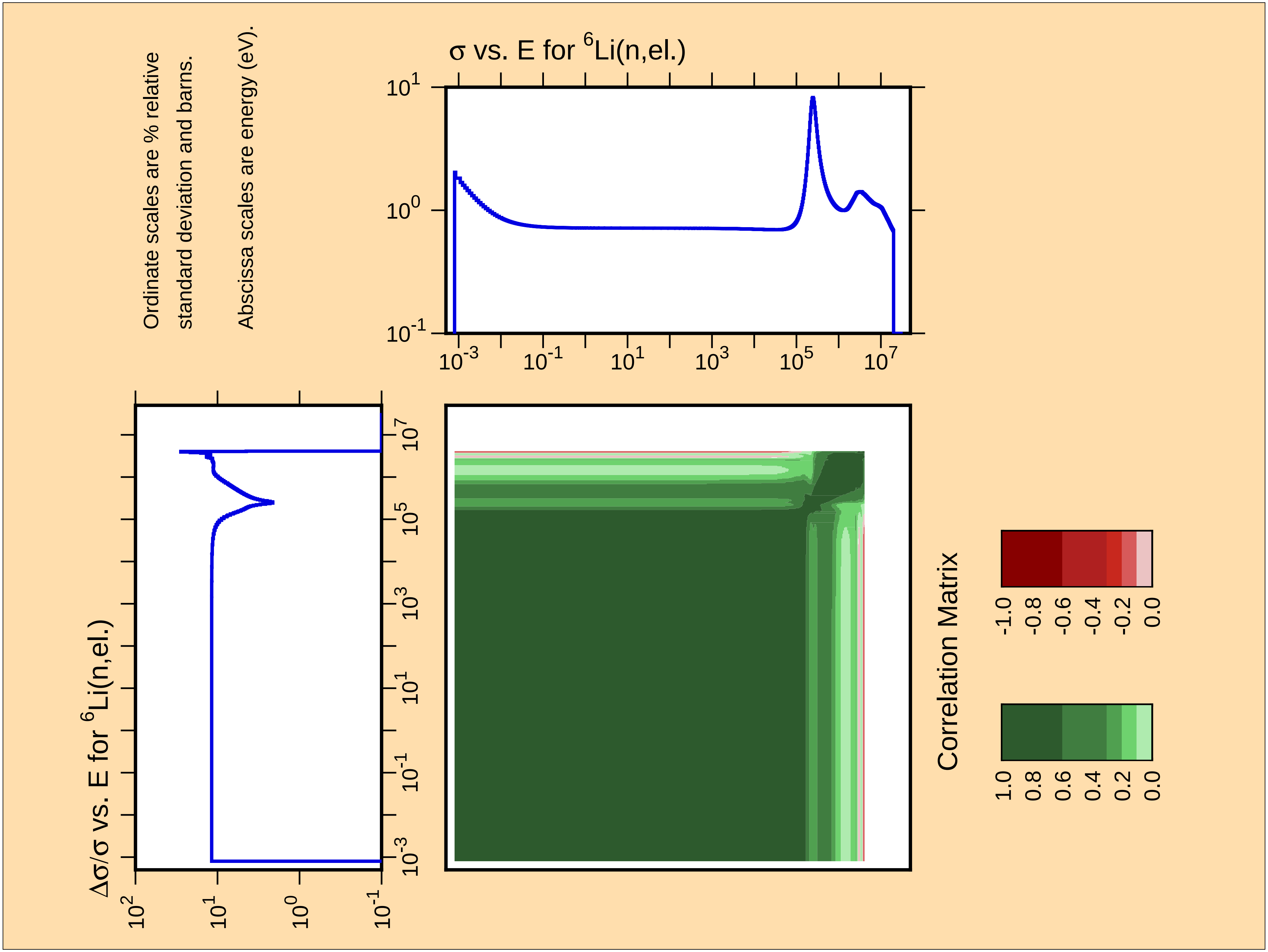

Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Δσ/σ vs. E for 1H(n,tot.)
1.0
0.8
0.6
0.4
0.2
0.0
10-3
10-1
101
103
105
107
Δσ/σ vs. E for 1H(n,el.)
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0


Δσ/σ vs. E for 1H(n,tot.)
Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Δσ/σ vs. E for 1H(n,γ)
Correlation Matrix
1.0
0.8
0.6
0.4
0.2
0.0
10-3
10-1
101
103
105
107
102
100
-1.0
-0.8
-0.6
-0.4
-0.2

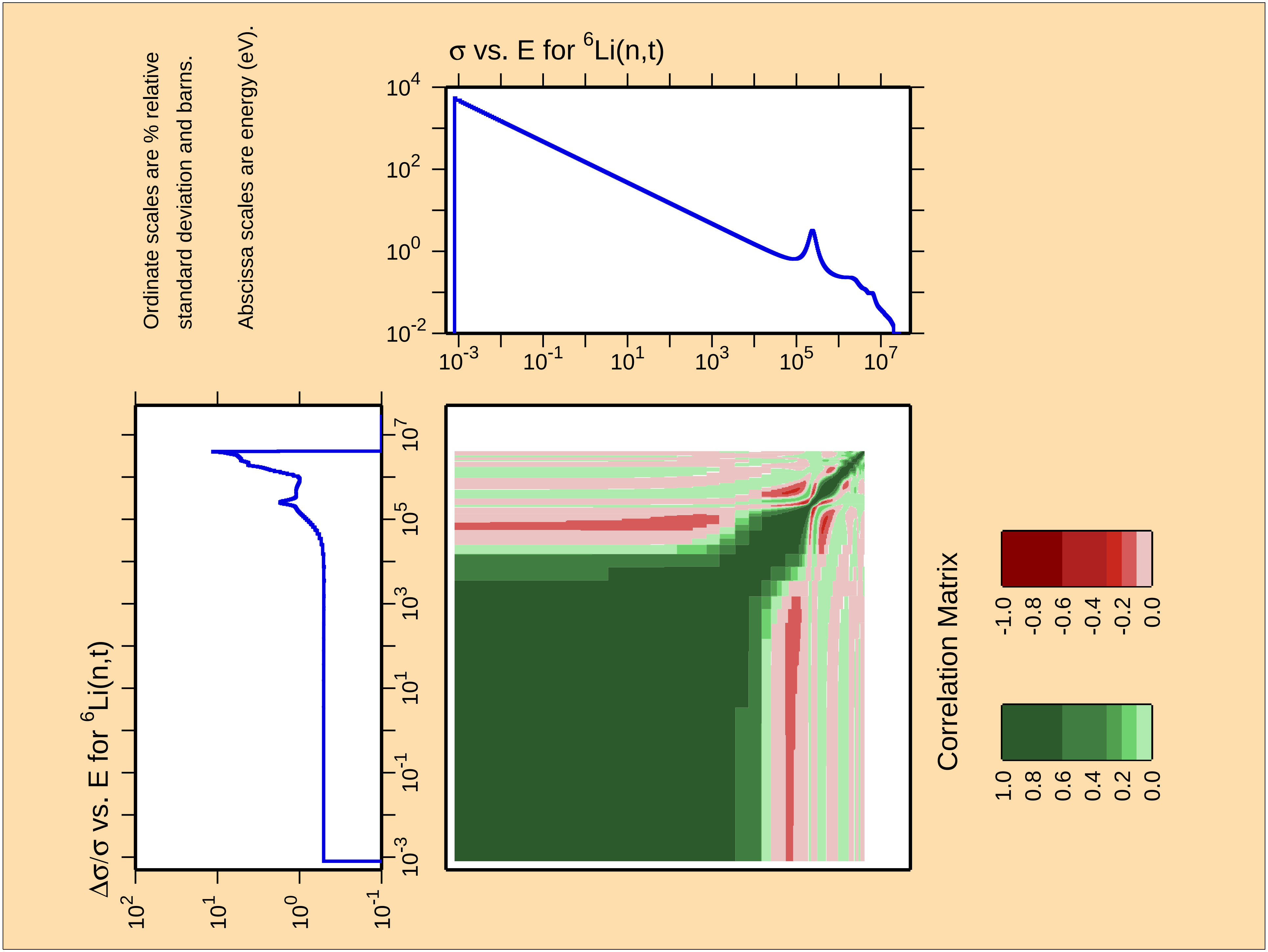

Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 1H(n,el.)
Δσ/σ vs. E for 1H(n,el.)
Correlation Matrix
1.0 0.8 0.6 0.4 0.2 0.0
-1.0 -0.8 -0.6 -0.4 -0.2 0.0



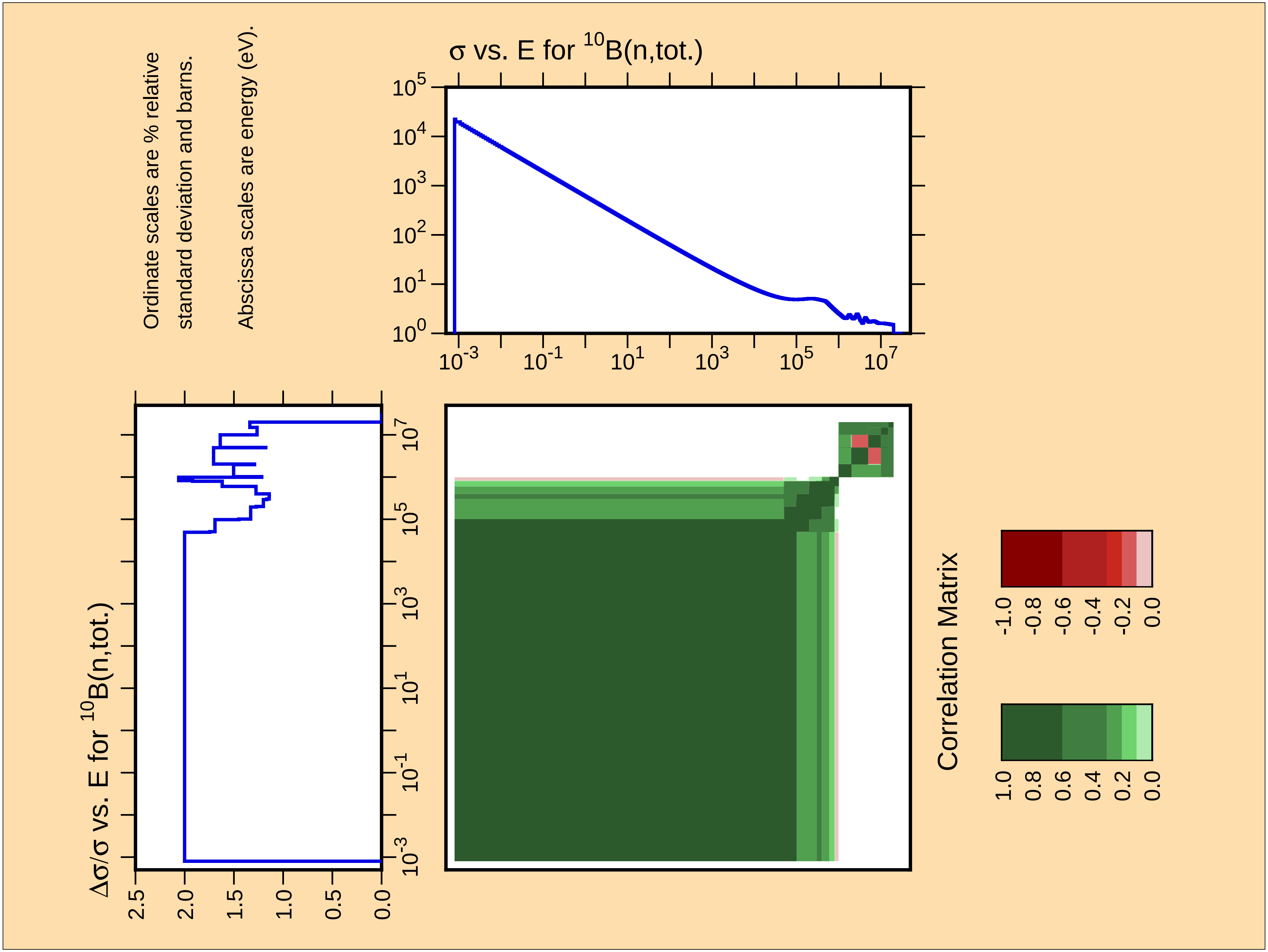
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for ¹H(n,γ)
10^1 10^-1 10^-3 10^-5
10^-3 10^-1 10^1 10^3 10^5 10^7
Δσ/σ vs. E for ¹H(n,γ)
10^2 10^1 10^0 10^-1
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0



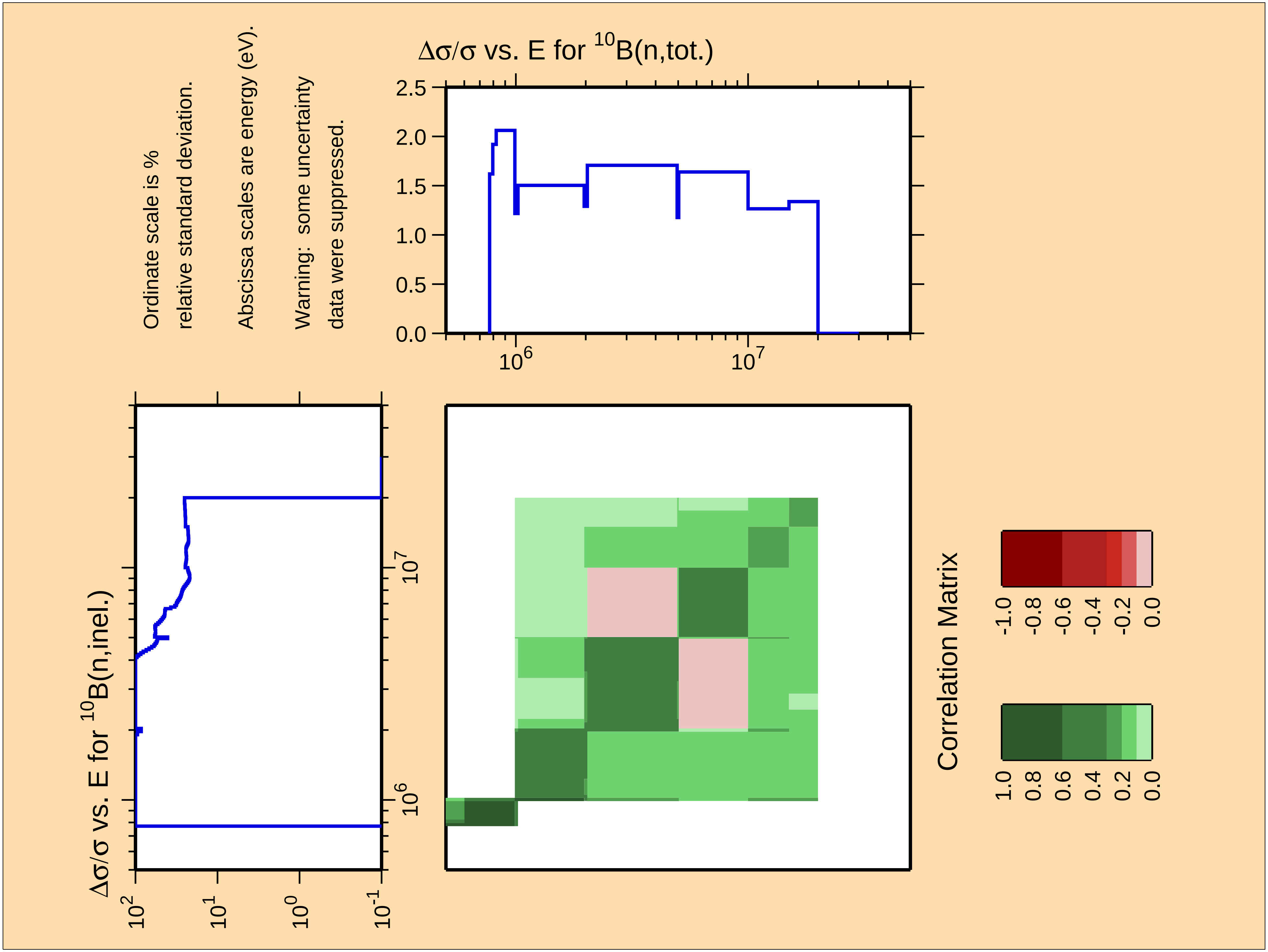
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 6Li(n,el.)
Δσ/σ vs. E for 6Li(n,el.)
Correlation Matrix



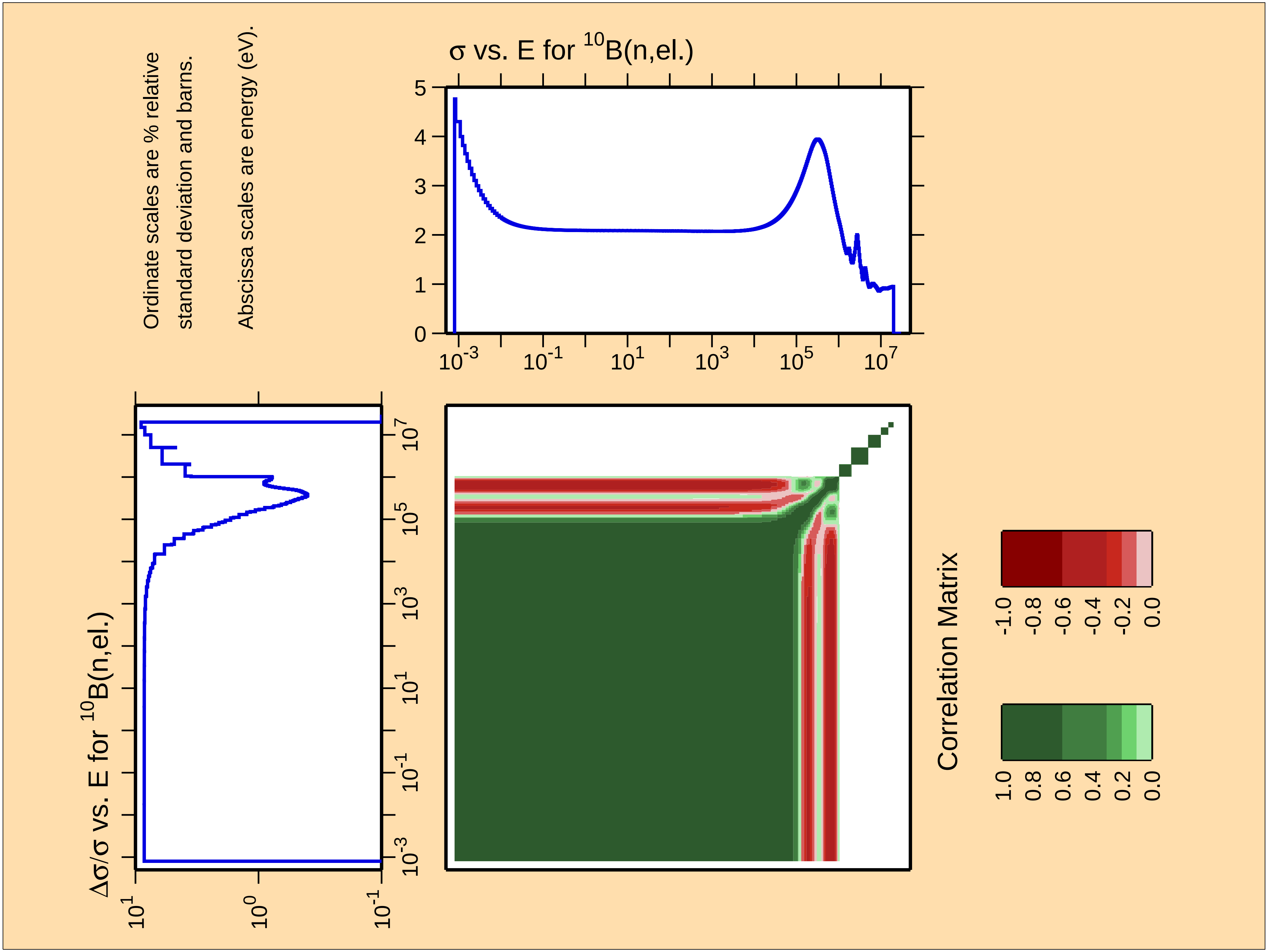
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 6Li(n,t)
Δσ/σ vs. E for 6Li(n,t)
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

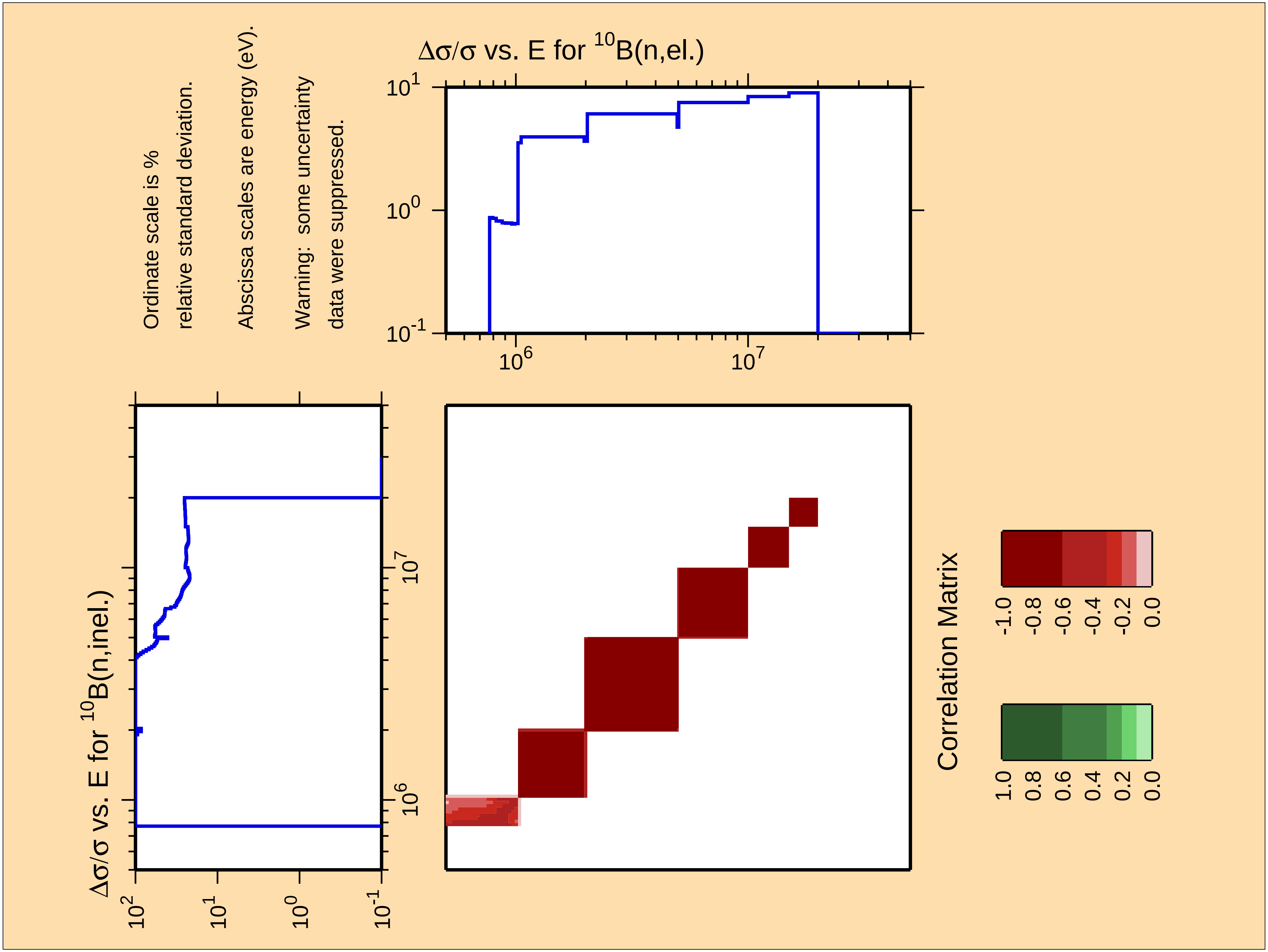


Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 10B(n,tot.)
Δσ/σ vs. E for 10B(n,tot.)
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

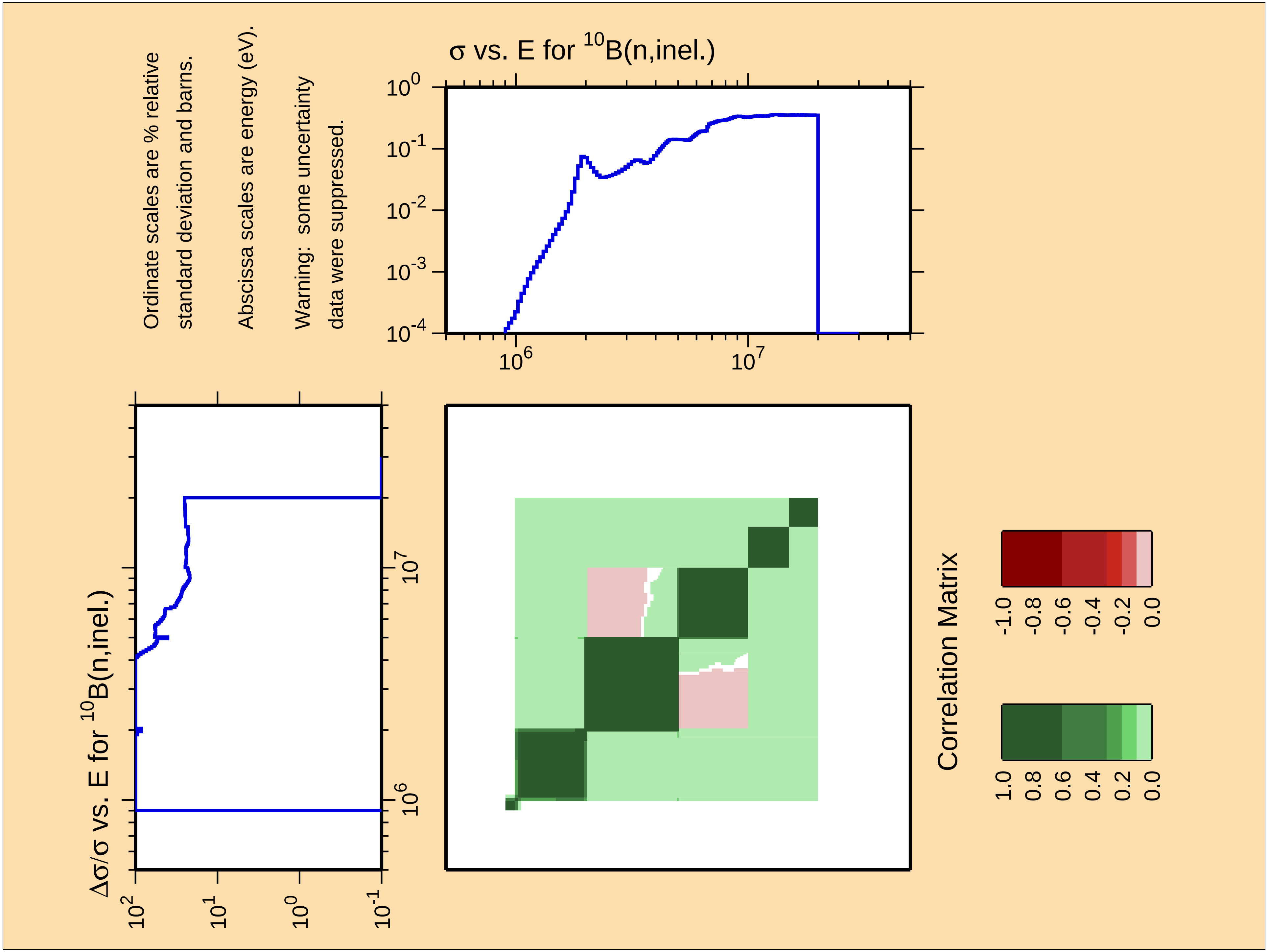


Δσ/σ vs. E for 10B(n,tot.)
Ordinate scale is % relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
Δσ/σ vs. E for 10B(n,inel.)
Correlation Matrix
2.5
2.0
1.5
1.0
0.5
0.0
10^6
10^7
10^2
10^1
10^0
10^-1
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

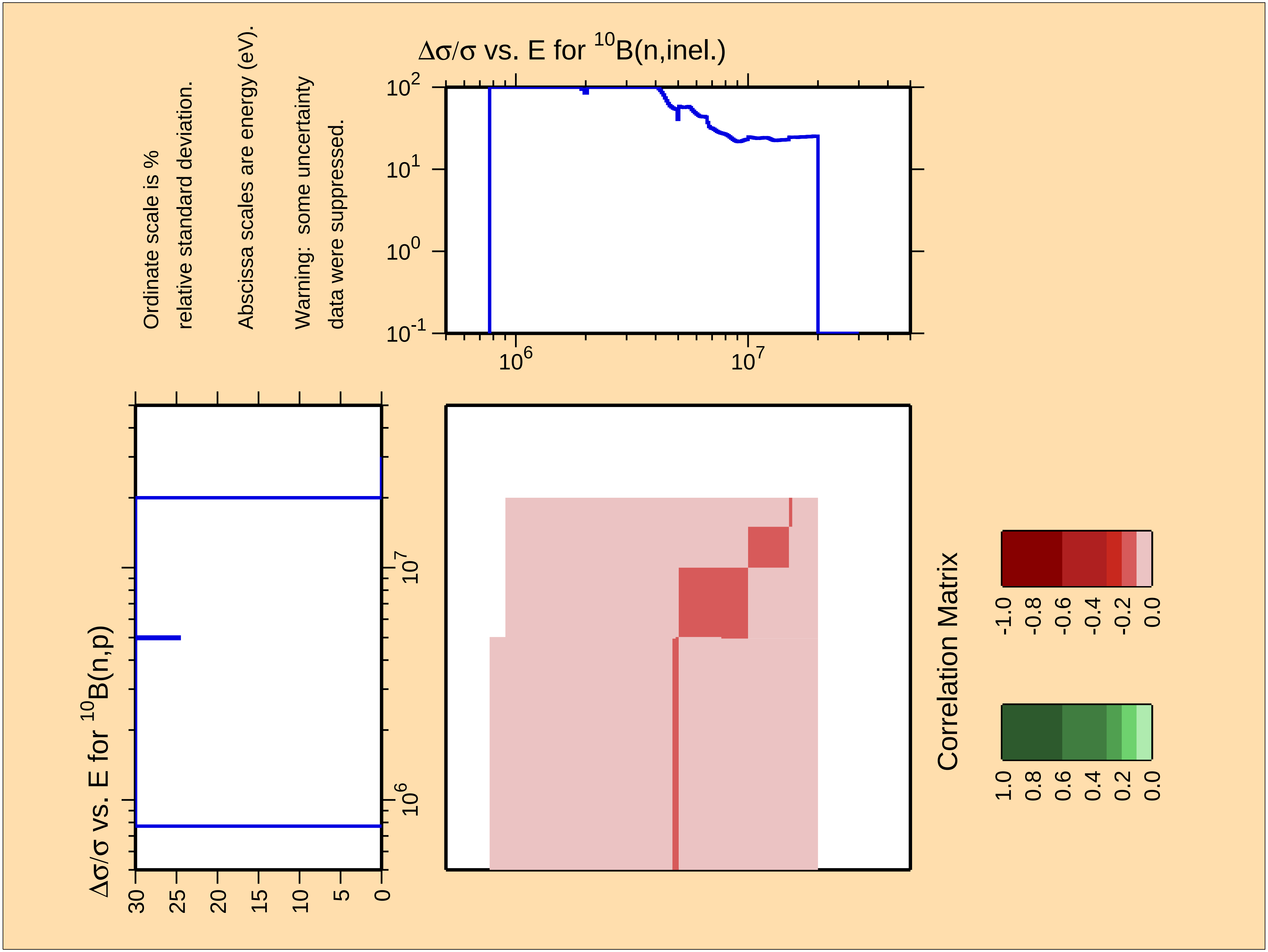

σ vs. E for 10B(n,el.)
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
Δσ/σ vs. E for 10B(n,el.)
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0



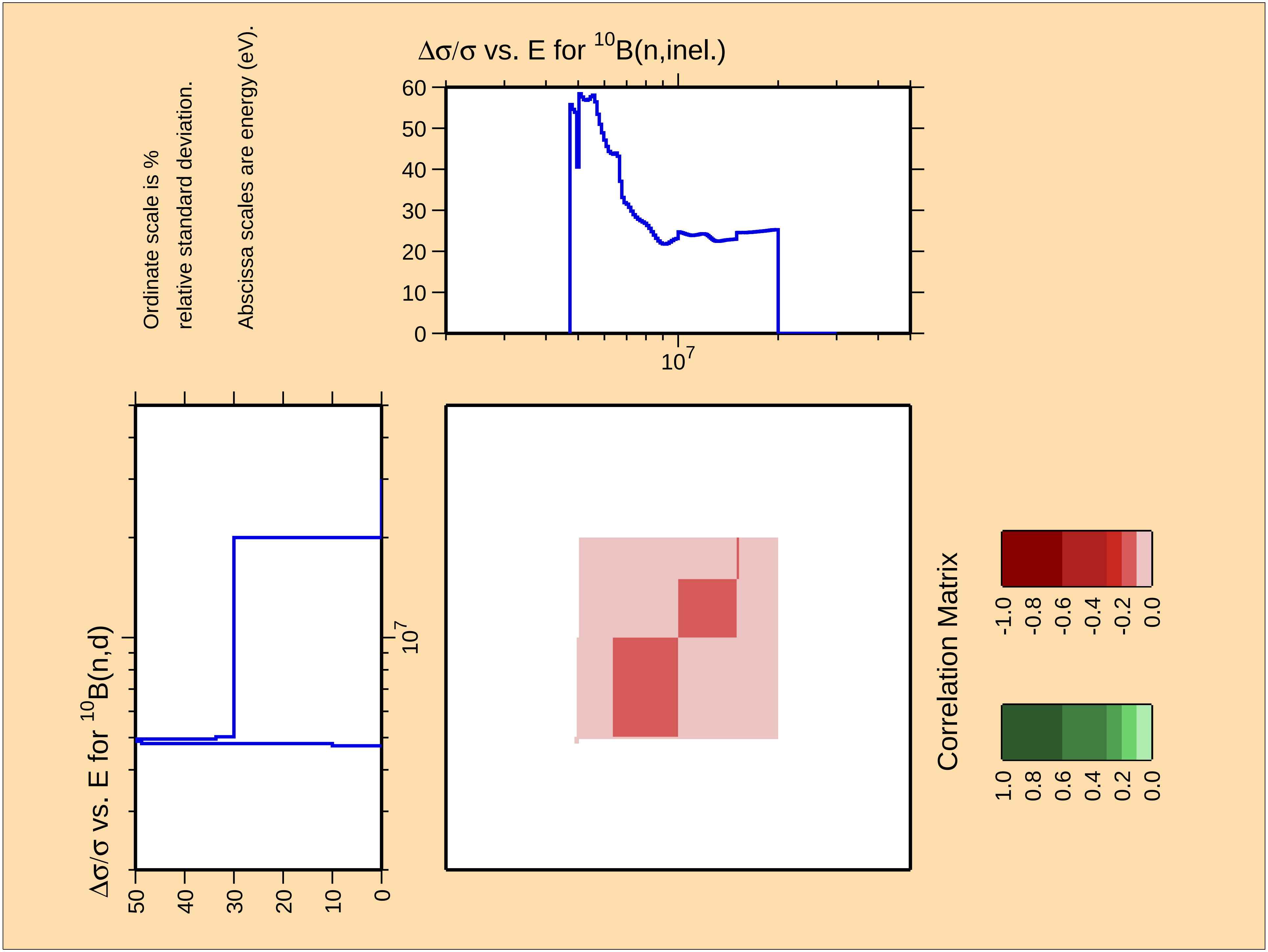
Δσ/σ vs. E for 10B(n,el.)
Ordinate scale is % relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
Δσ/σ vs. E for 10B(n,inel.)
Correlation Matrix
10^1
10^0
10^-1
10^6
10^7
10^2
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0



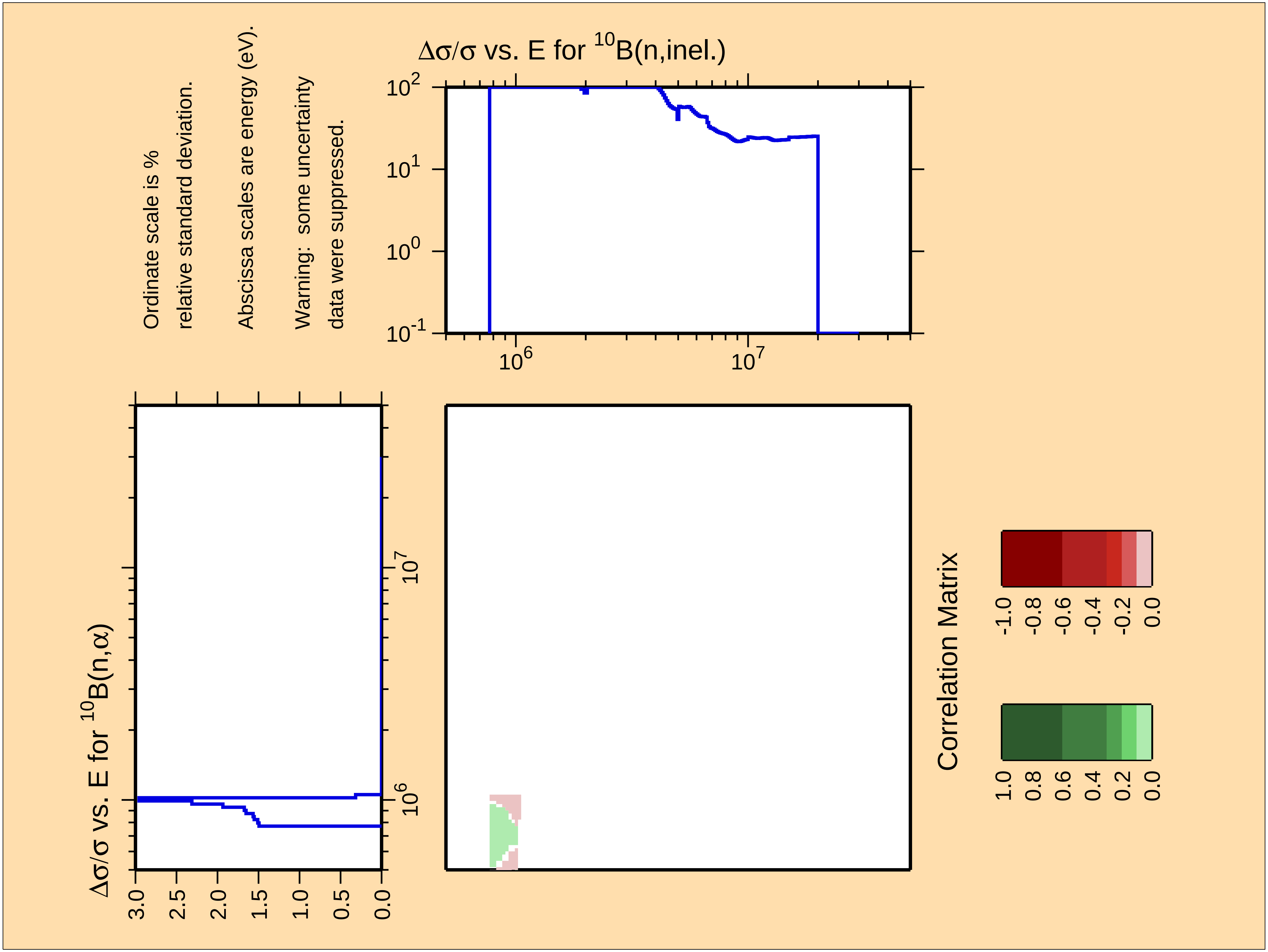
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
σ vs. E for 10B(n,inel.)
10^0
10^-1
10^-2
10^-3
10^-4
10^6
10^7
Δσ/σ vs. E for 10B(n,inel.)
10^2
10^1
10^0
10^-1
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

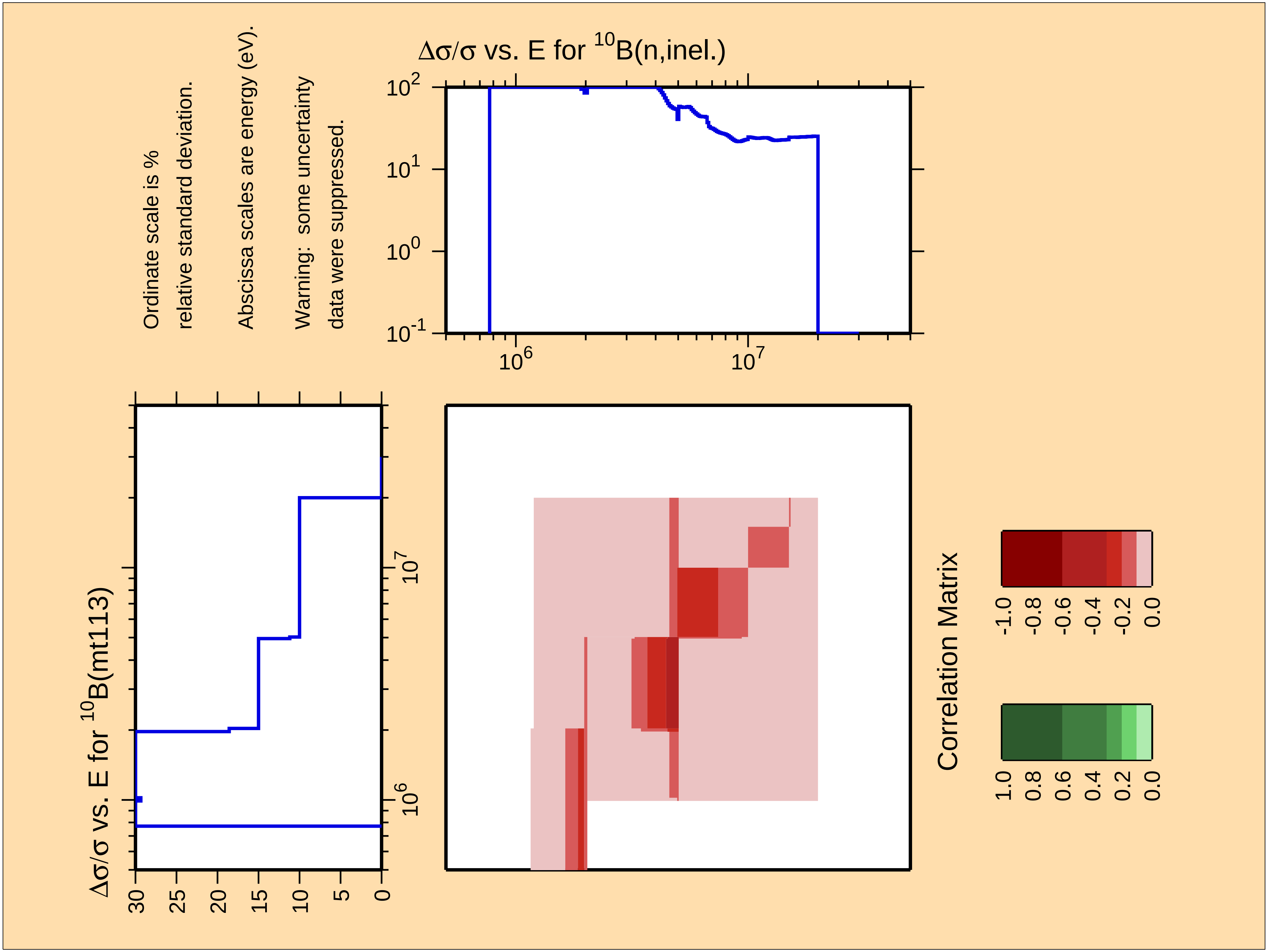


Δσ/σ vs. E for 10B(n,inel.)
Ordinate scale is % relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
Δσ/σ vs. E for 10B(n,p)
Correlation Matrix
10^2
10^1
10^0
10^-1
10^6
10^7
30
25
20
15
10
5
0
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

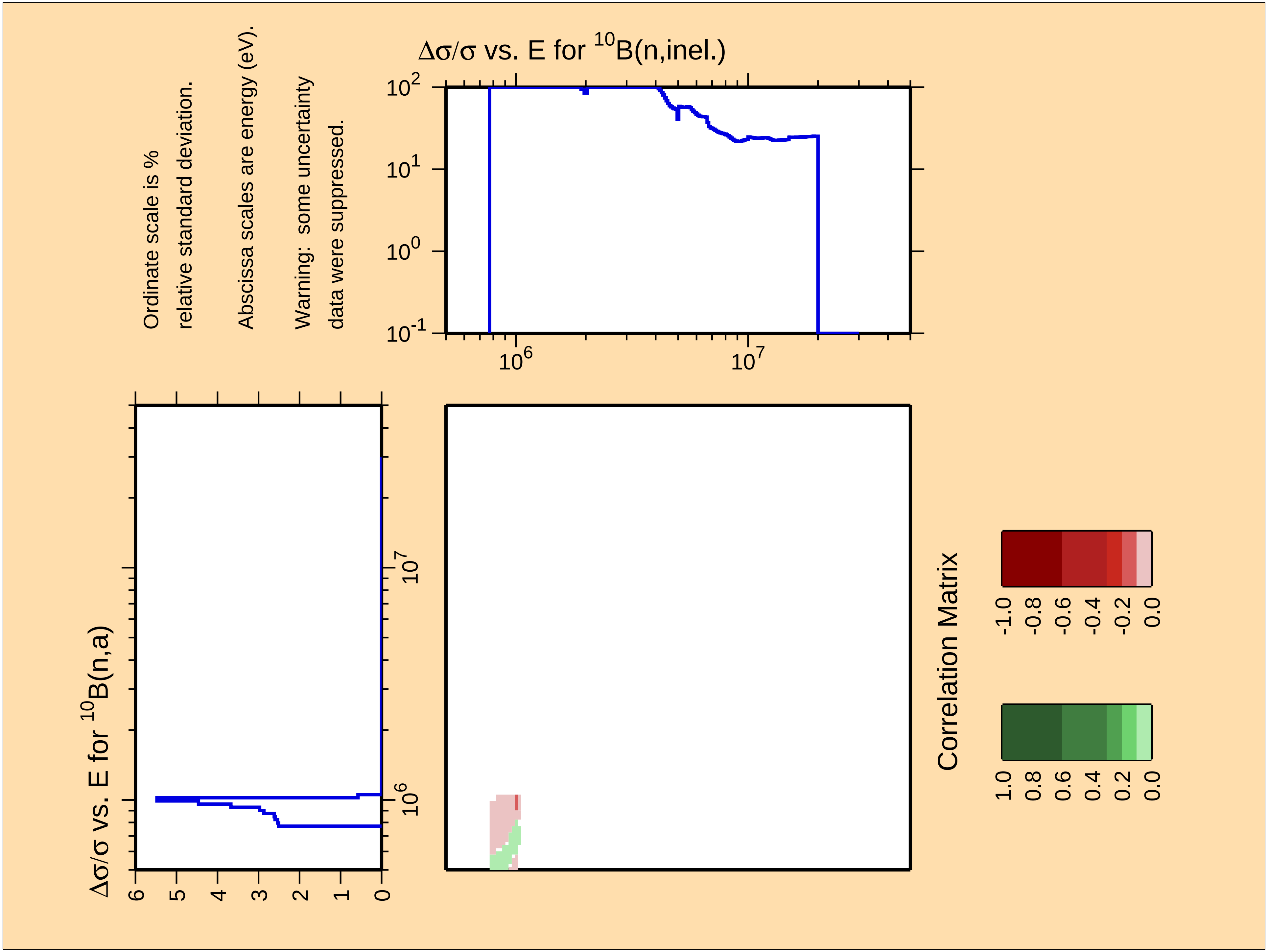


Δσ/σ vs. E for 10B(n,inel.)
Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
60
50
40
30
20
10
0
10^7
Δσ/σ vs. E for 10B(n,d)
50
40
30
20
10
0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0

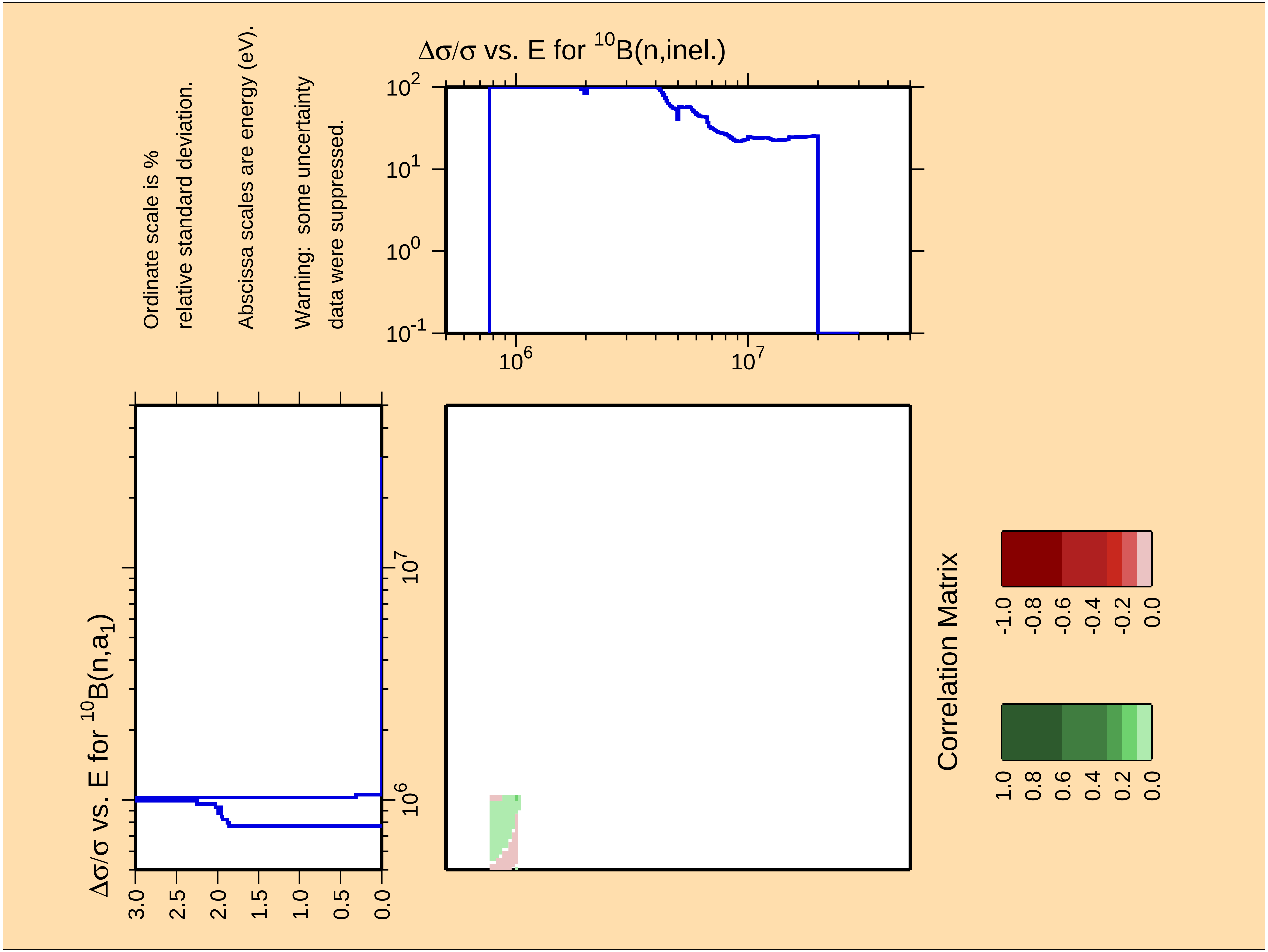

Δσ/σ vs. E for 10B(n,inel.)
Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty
data were suppressed.
10^2
10^1
10^0
10^-1
10^6
10^7
Δσ/σ vs. E for 10B(n,α)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0



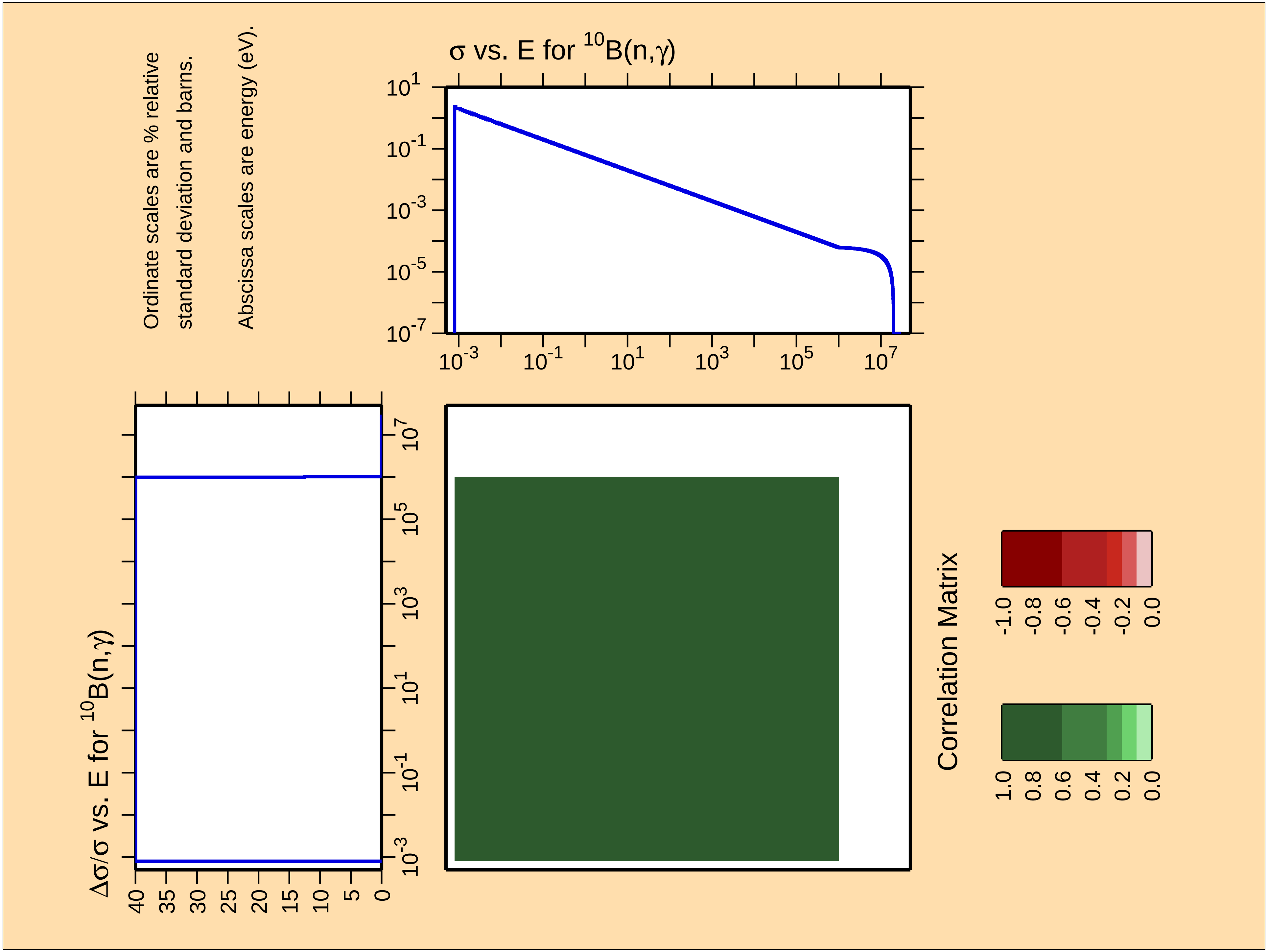
Δσ/σ vs. E for 10B(n,inel.)
Ordinate scale is % relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
10^2
10^1
10^0
10^-1
10^6
10^7
Δσ/σ vs. E for 10B(mt113)
30
25
20
15
10
5
0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2



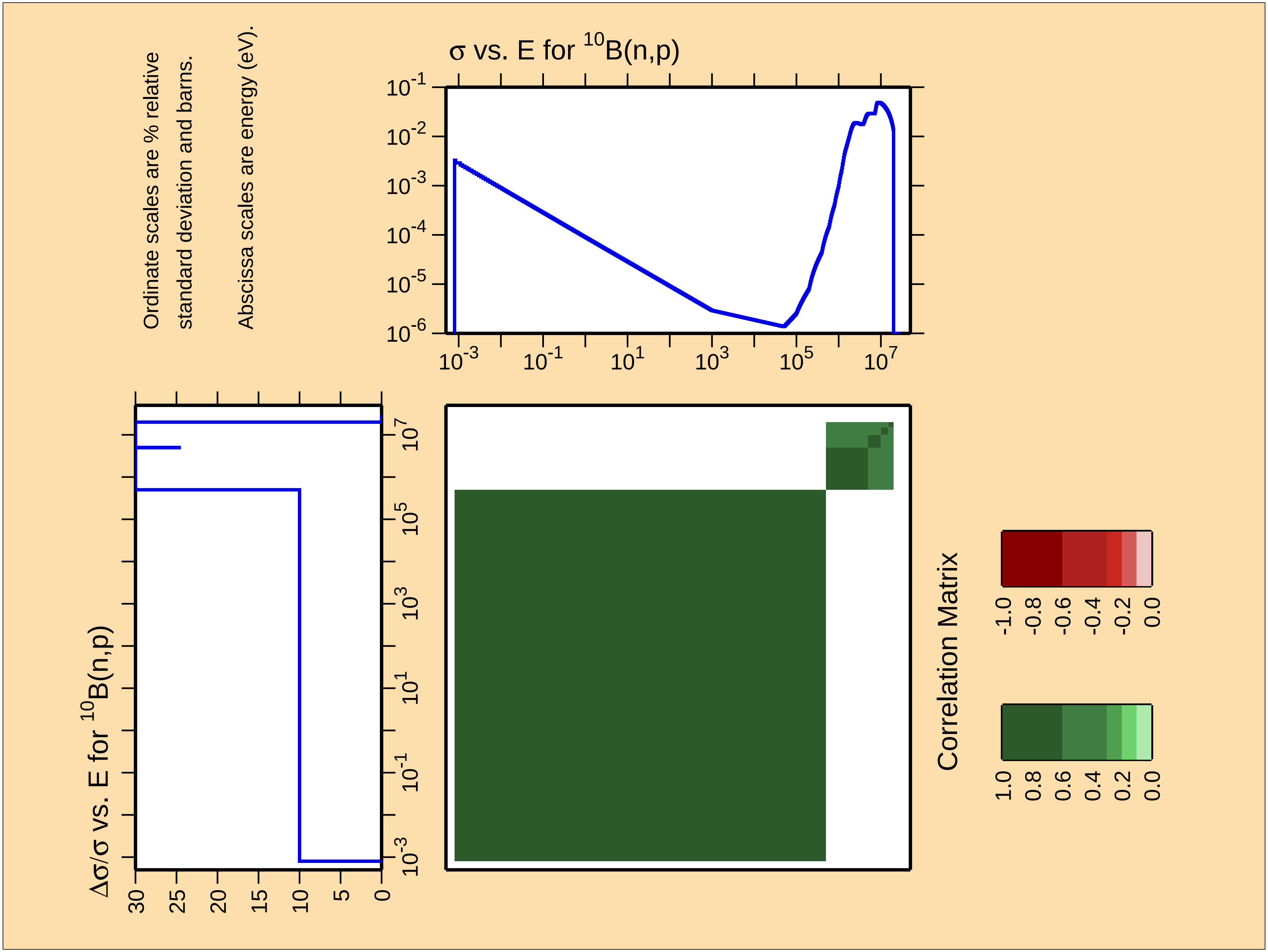
Δσ/σ vs. E for 10B(n,inel.)
Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty
data were suppressed.
10^2
10^1
10^0
10^-1
10^6
10^7
Δσ/σ vs. E for 10B(n,a)
6 5 4 3 2 1 0
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

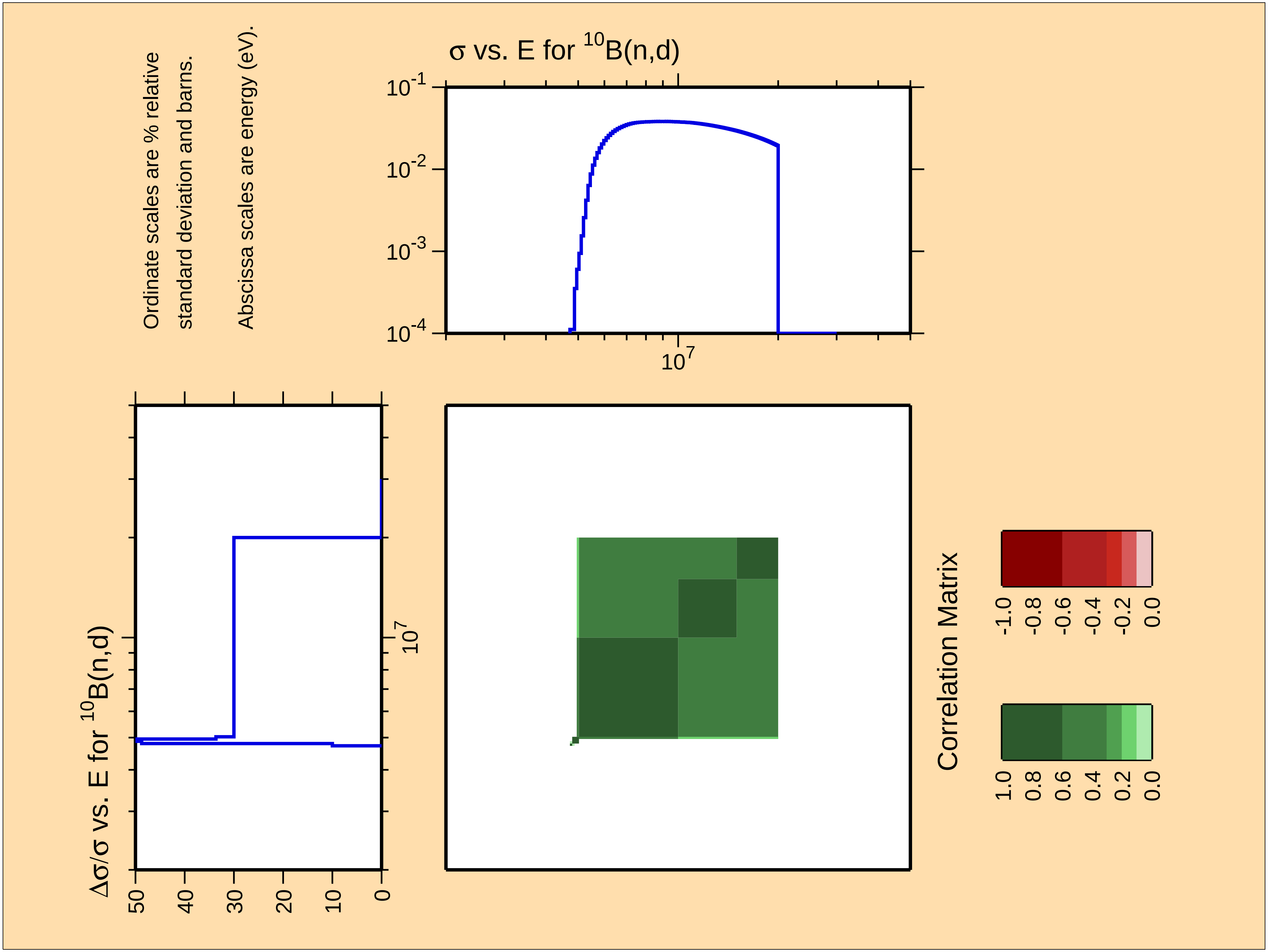


Δσ/σ vs. E for 10B(n,inel.)
Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Warning: some uncertainty
data were suppressed.
Δσ/σ vs. E for 10B(n,a1)
Correlation Matrix
10-1
10 0
10 1
10 2
10 6
10 7
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0

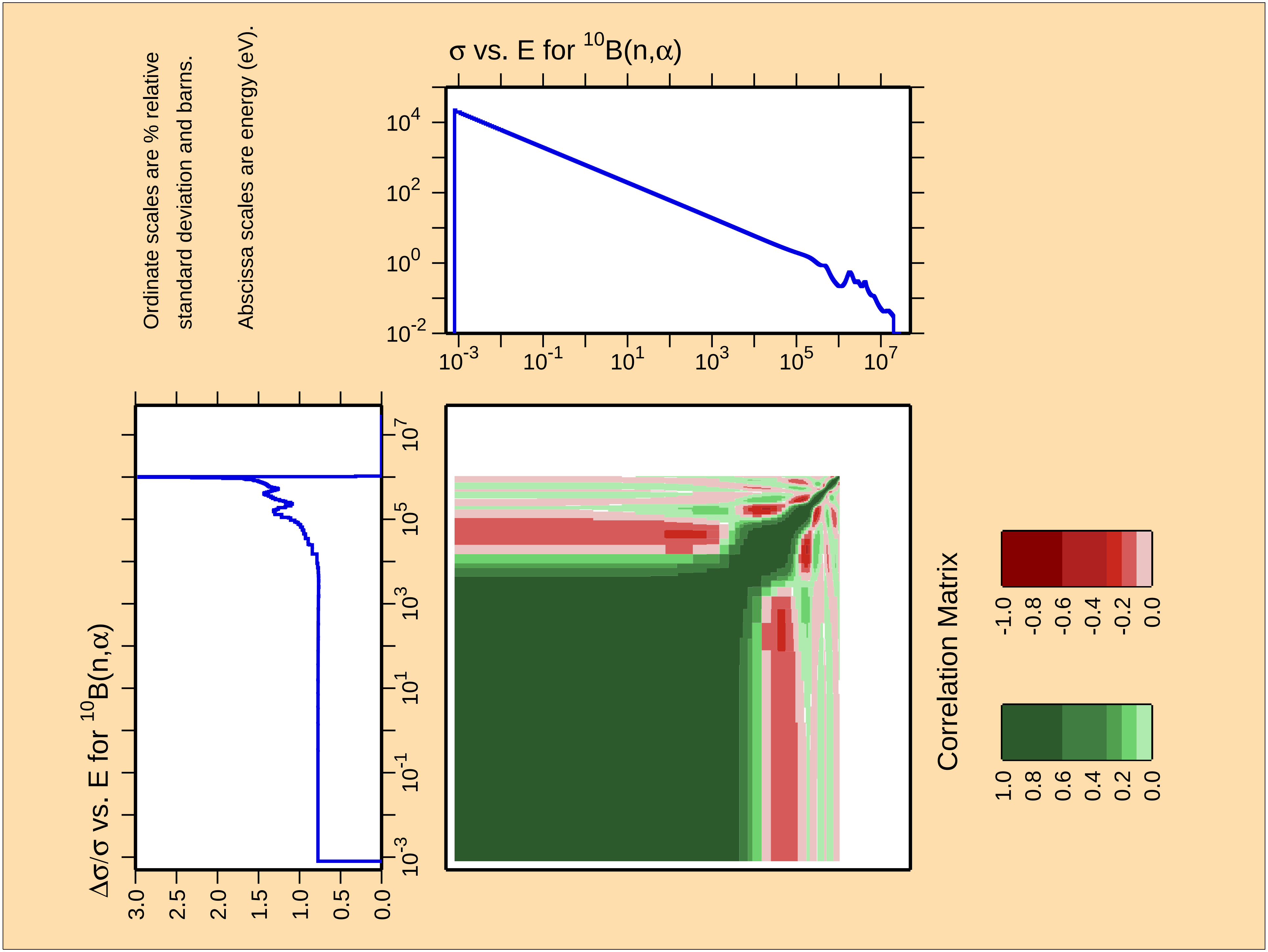


Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 10B(n,γ)
10^1
10^-1
10^-3
10^-5
10^-7
10^-3
10^-1
10^1
10^3
10^5
10^7
Δσ/σ vs. E for 10B(n,γ)
40
35
30
25
20
15
10
5
0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0

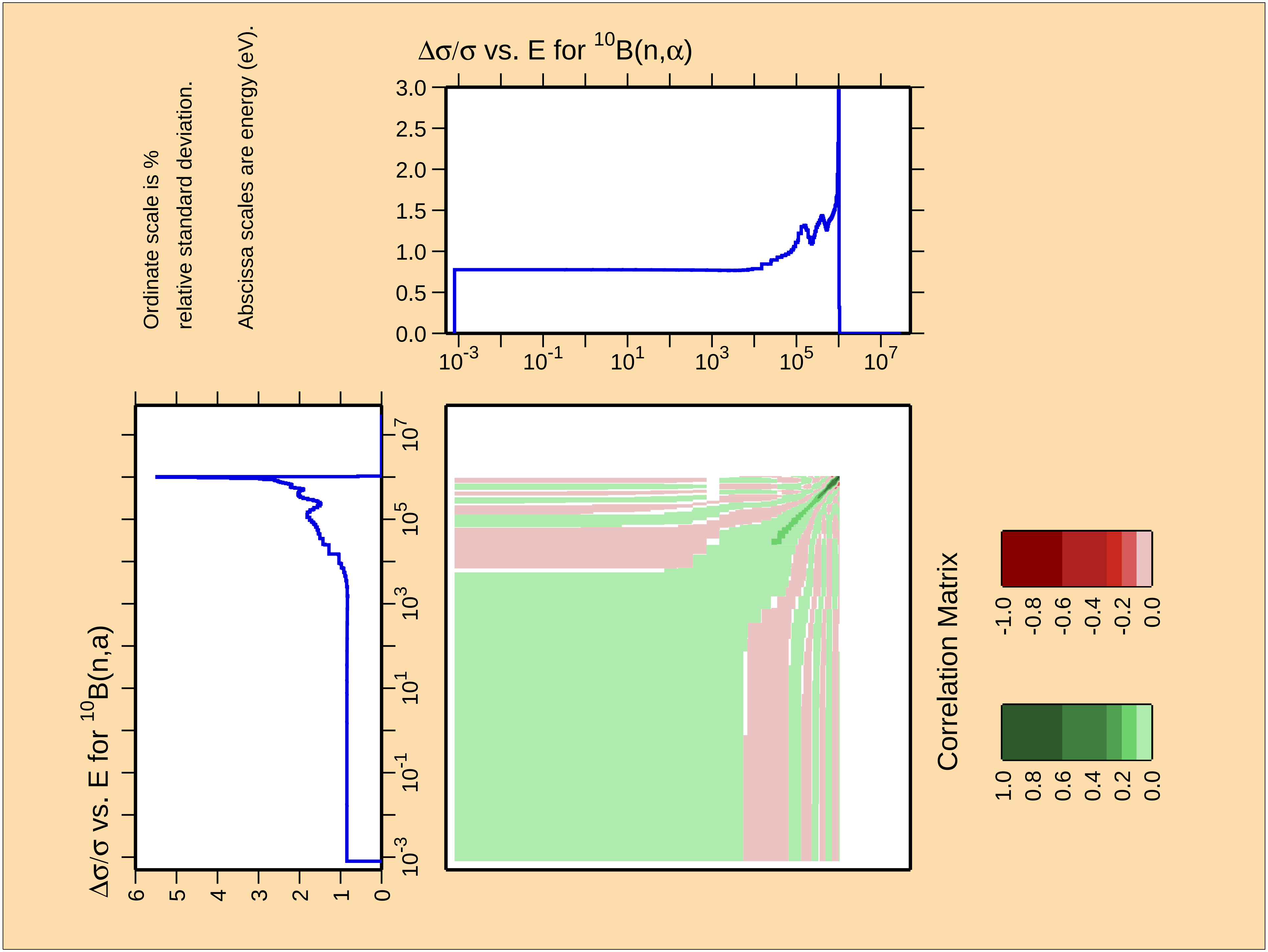

Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 10B(n,p)
Δσ/σ vs. E for 10B(n,p)
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0

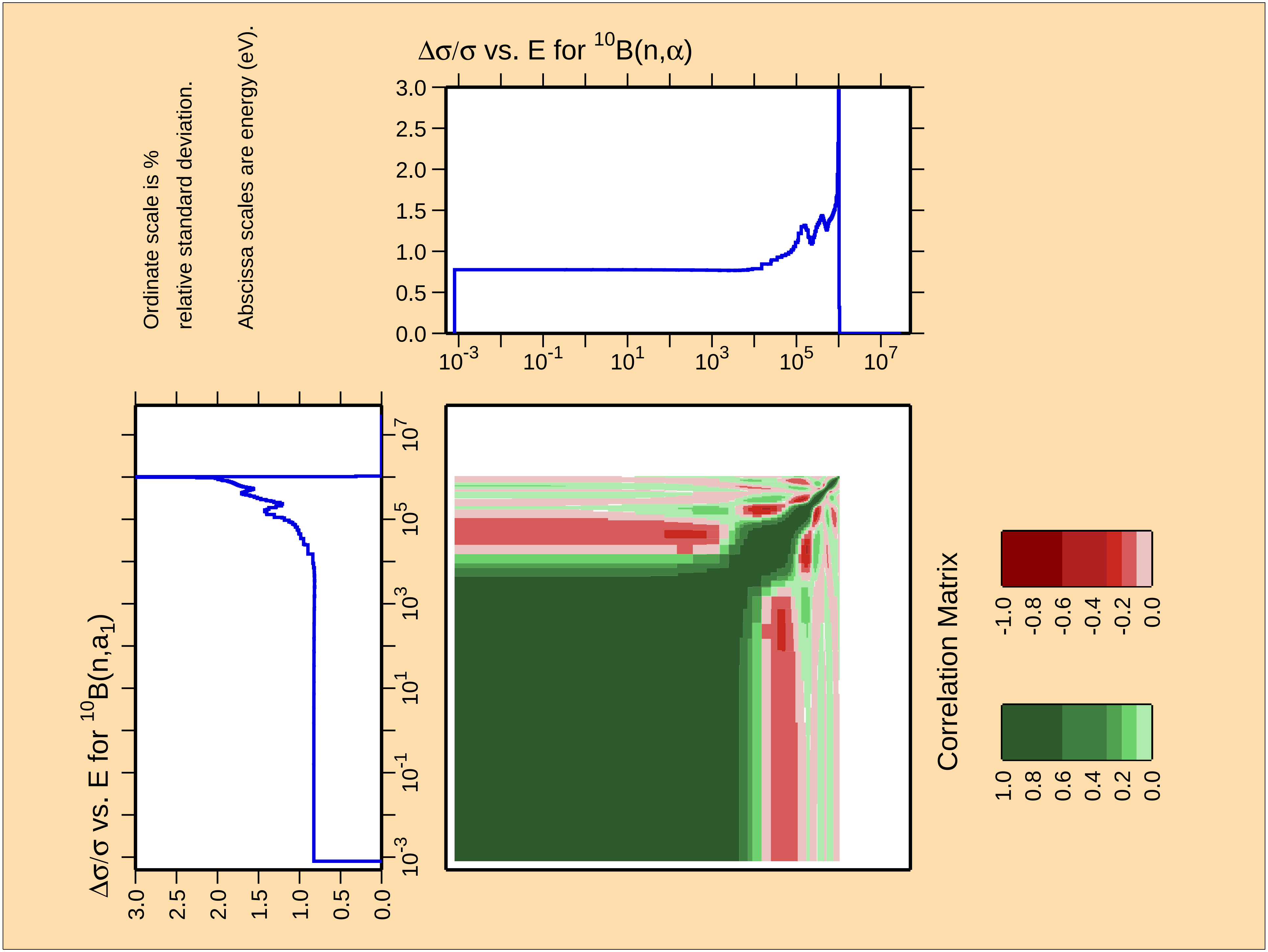


Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 10B(n,d)
10-1
10-2
10-3
10-4
107
Δσ/σ vs. E for 10B(n,d)
50
40
30
20
10
0
107
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0

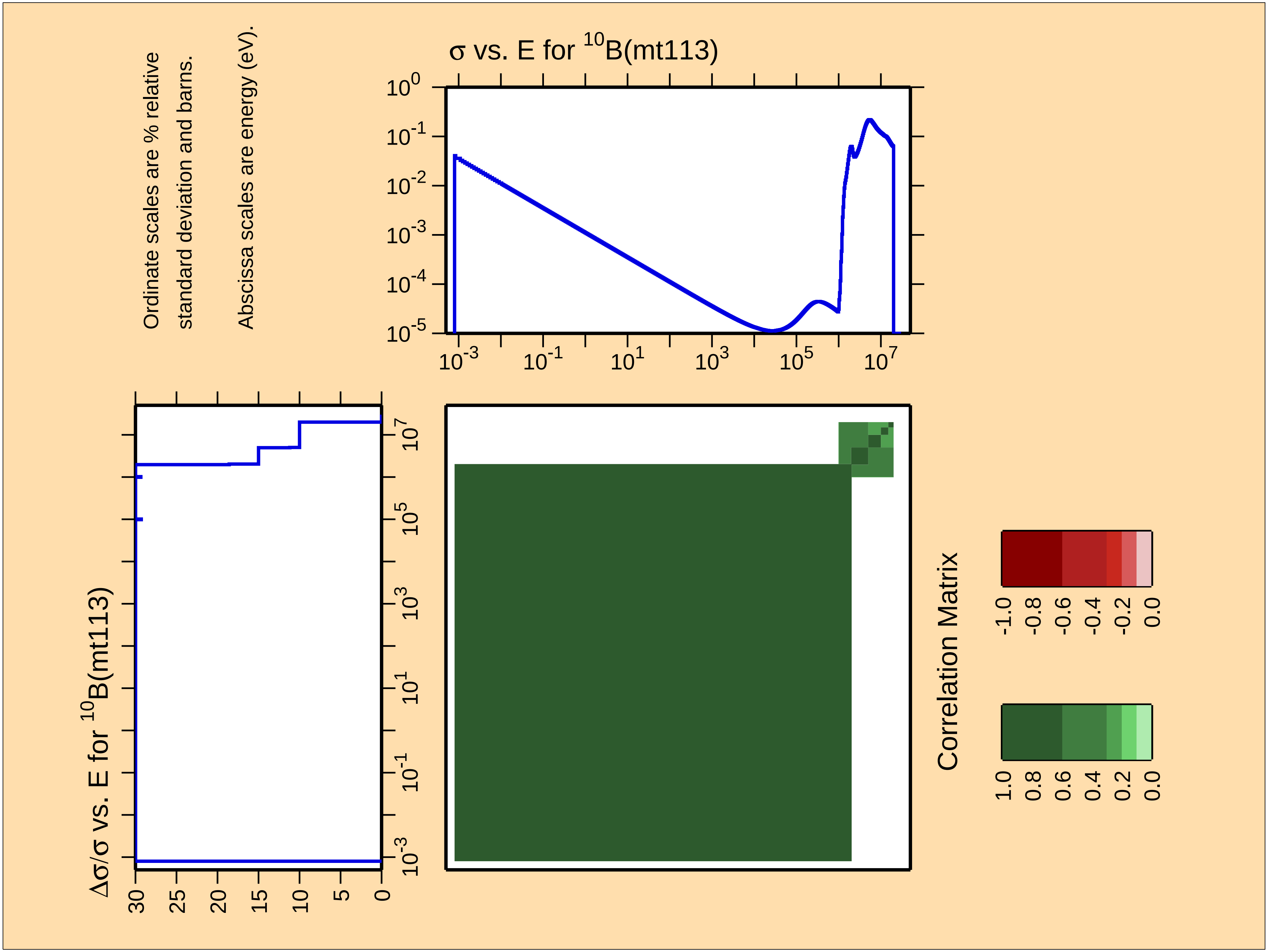


Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 10B(n,α)
10^{4}
10^{2}
10^{0}
10^{-2}
10^{-3}
10^{-1}
10^{1}
10^{3}
10^{5}
10^{7}
Δσ/σ vs. E for 10B(n,α)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0

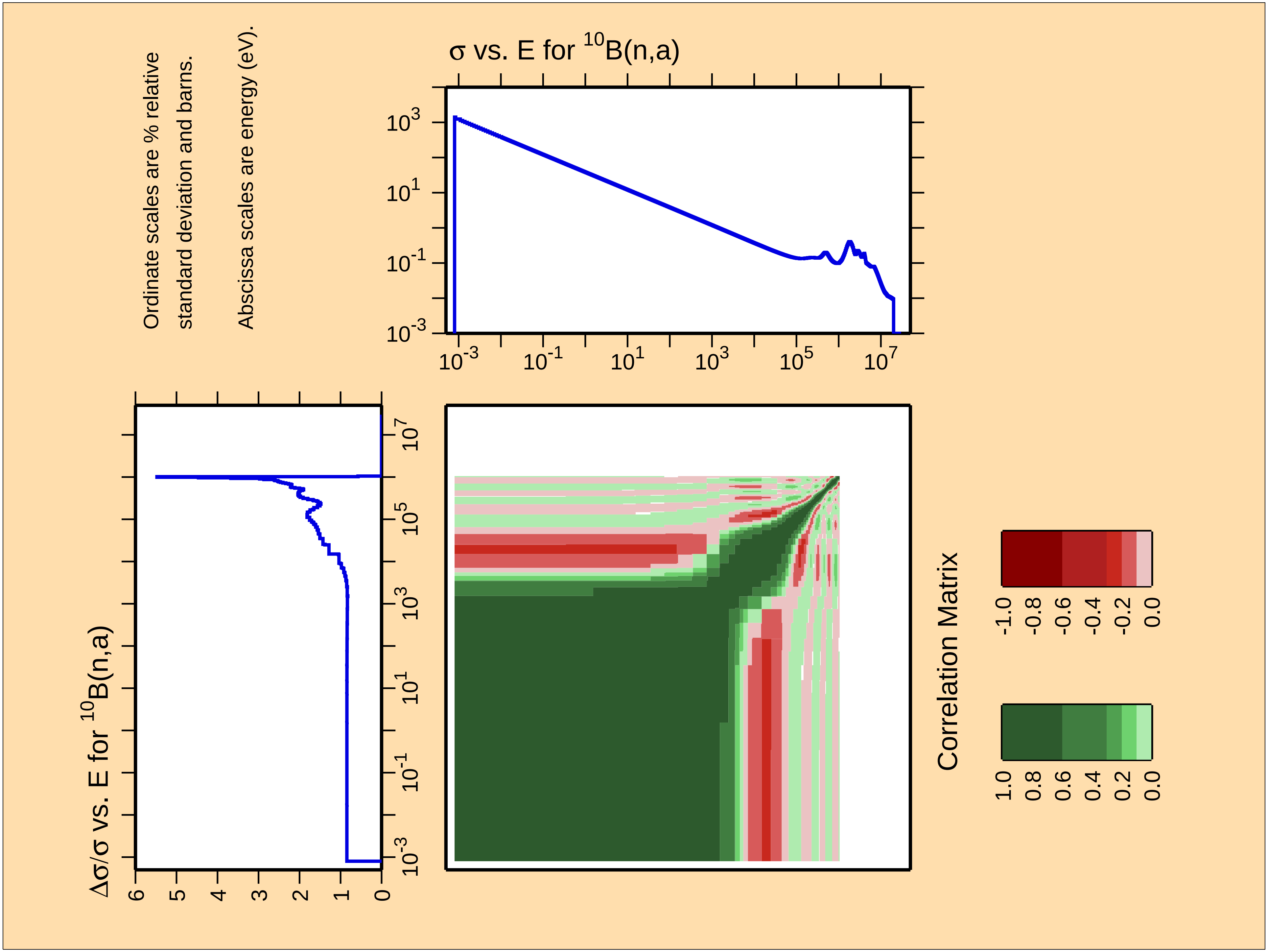

Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Δσ/σ vs. E for ^{10}B(n,α)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
10^{-3}
10^{-1}
10^{1}
10^{3}
10^{5}
10^{7}
Δσ/σ vs. E for ^{10}B(n,a)
6
5
4
3
2
1
0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0



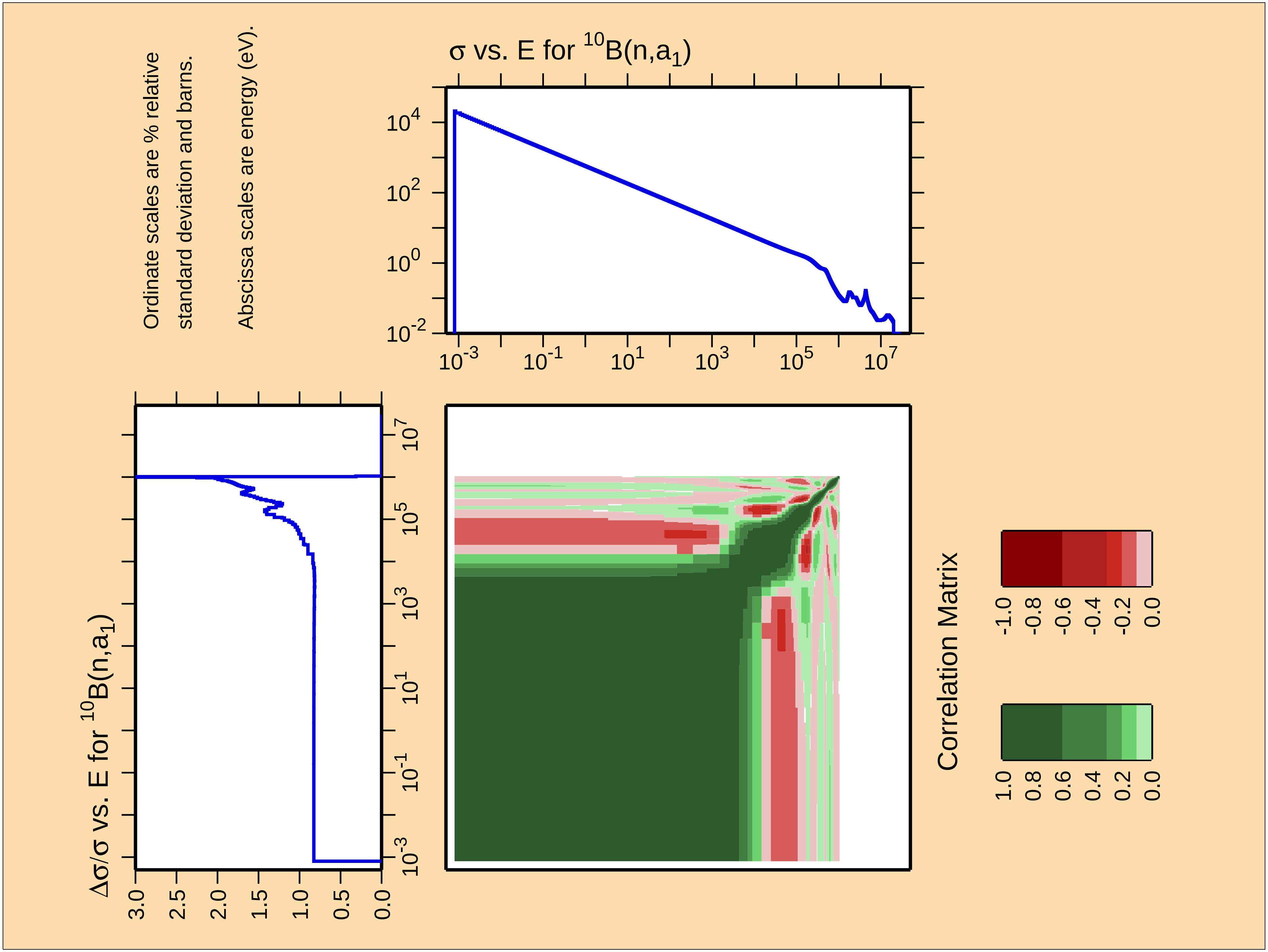
Δσ/σ vs. E for 10B(n,α)
Ordinate scale is %
relative standard deviation.
Abscissa scales are energy (eV).
Δσ/σ vs. E for 10B(n,a1)
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0



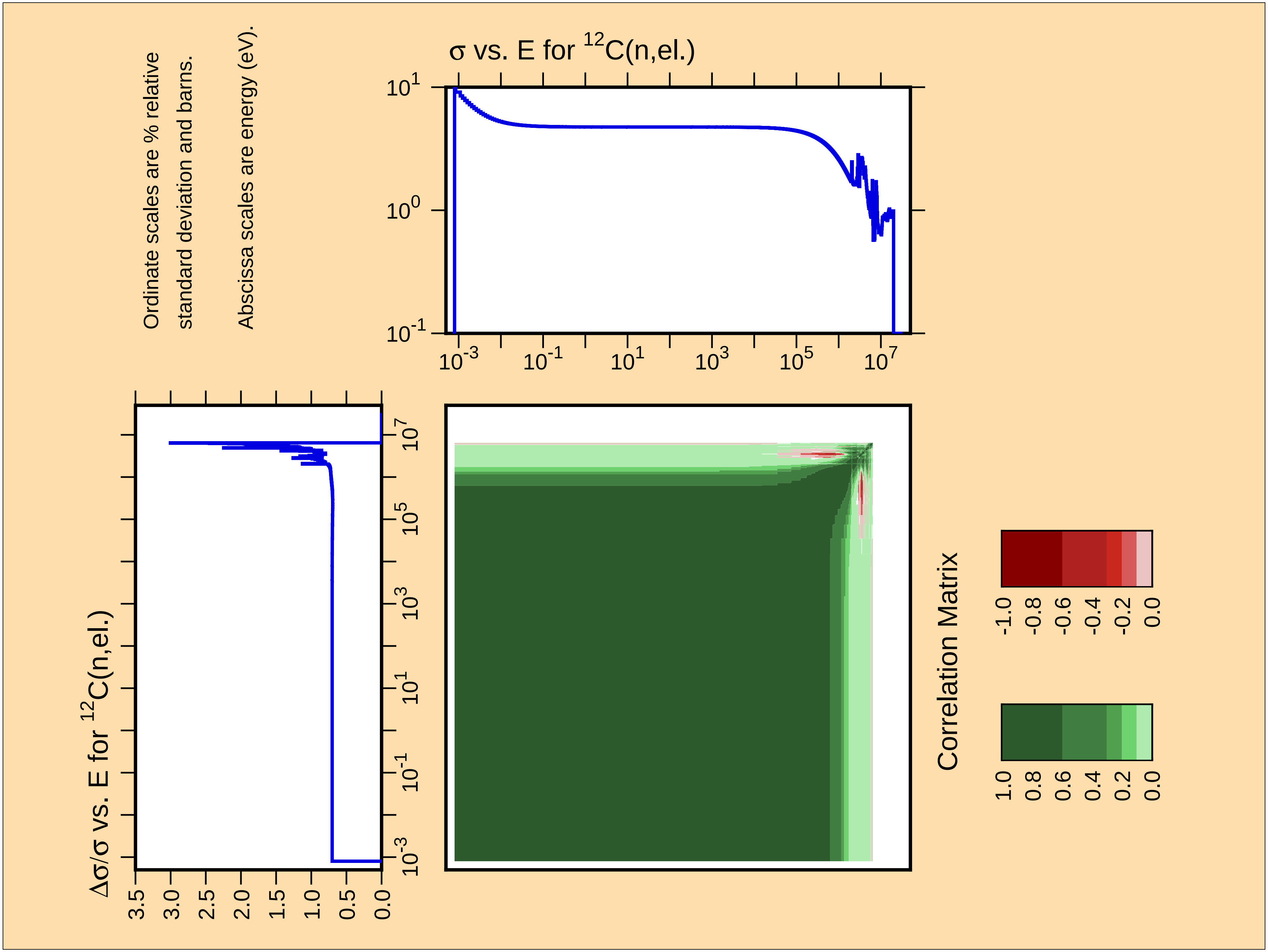
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for ^{10}B(mt113)
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-3}
10^{-1}
10^{1}
10^{3}
10^{5}
10^{7}
Δσ/σ vs. E for ^{10}B(mt113)
30
25
20
15
10
5
0
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0



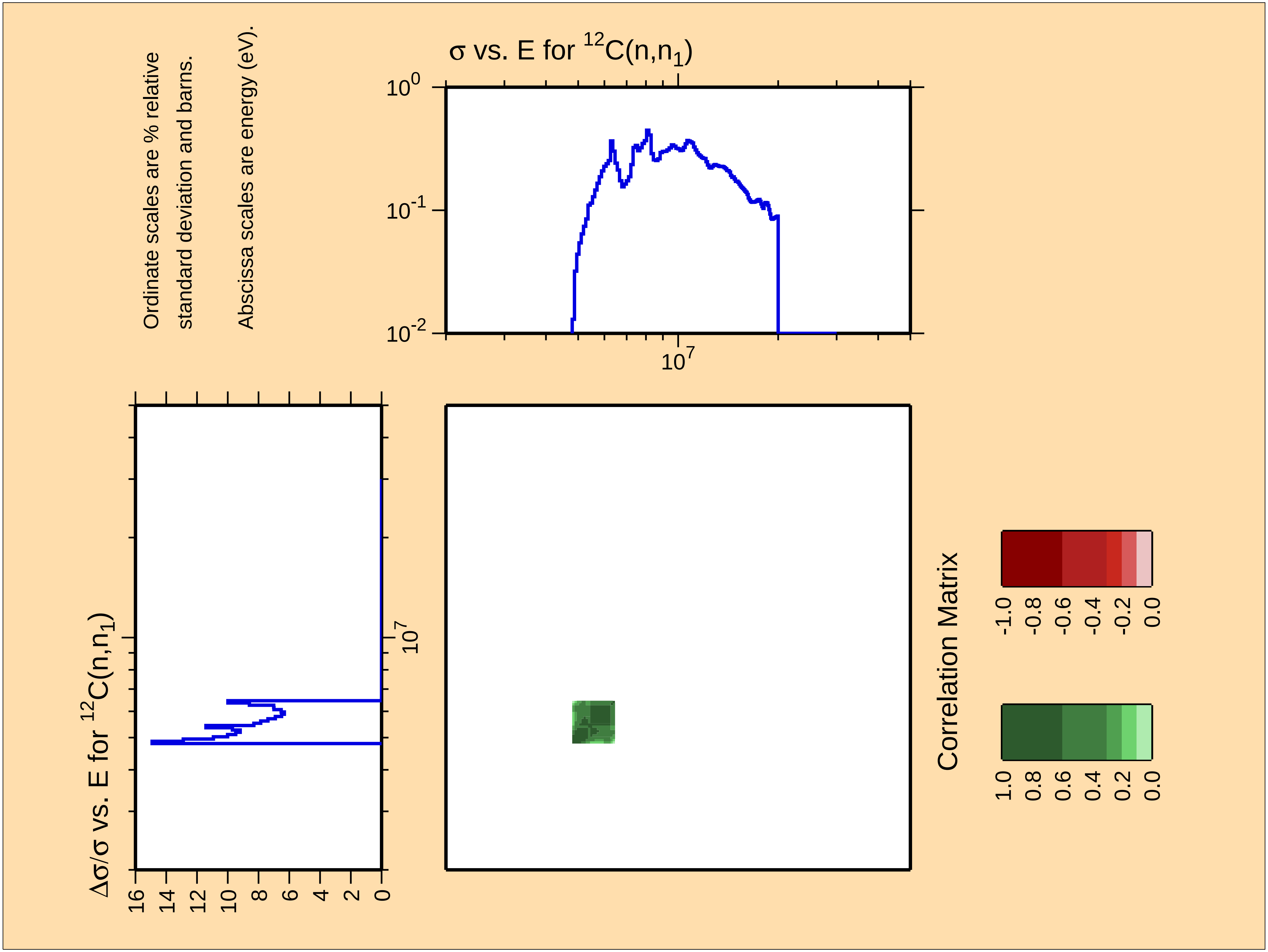
σ vs. E for 10B(n,a)
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
Δσ/σ vs. E for 10B(n,a)
Correlation Matrix



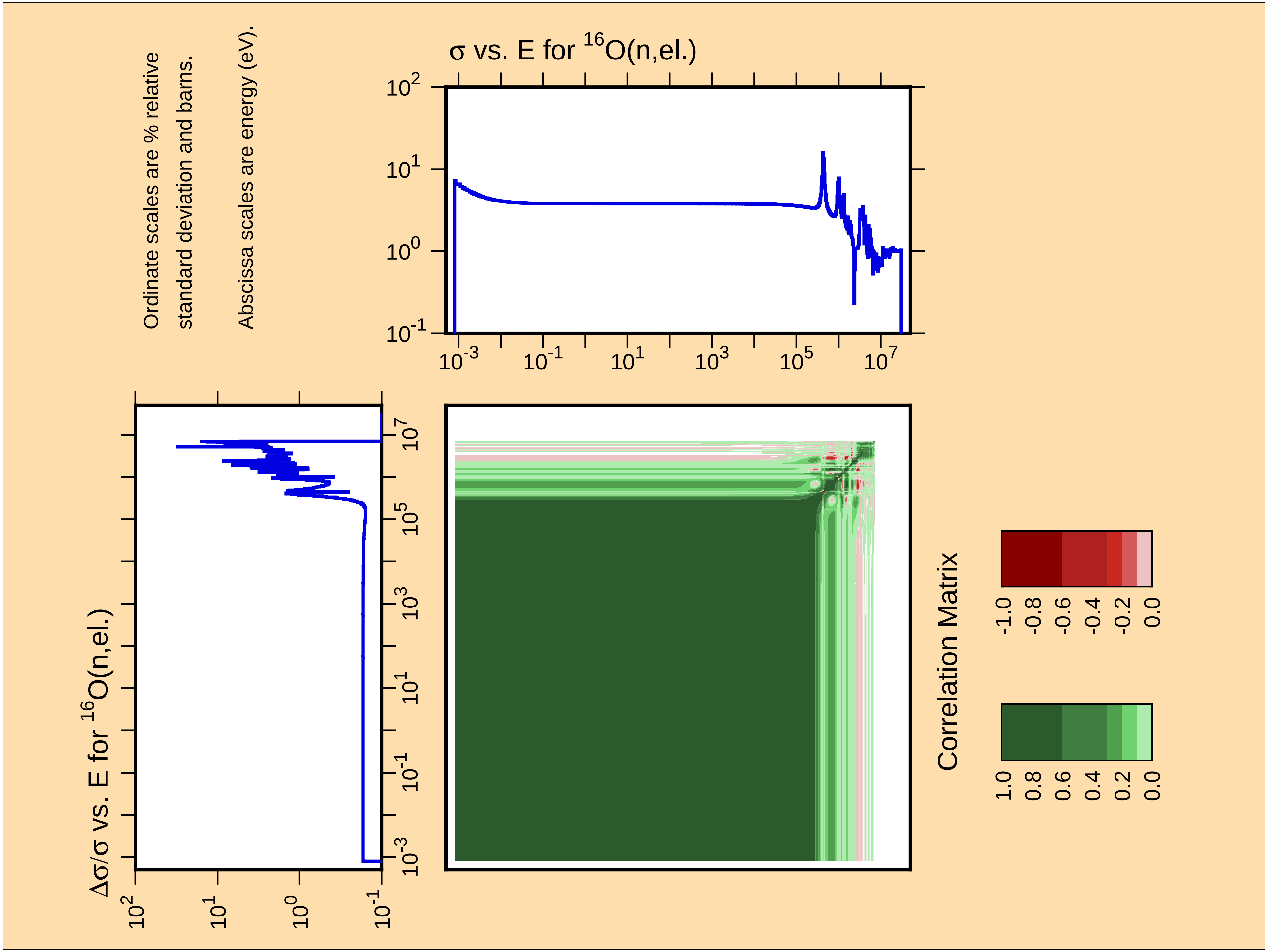
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for ^{10}B(n,a$_1$)
10^4
10^2
10^0
10^{-2}
10^{-3} 10^{-1} 10^1 10^3 10^5 10^7
Δσ/σ vs. E for ^{10}B(n,a$_1$)
3.0 2.5 2.0 1.5 1.0 0.5 0.0
10^{-3} 10^{-1} 10^1 10^3 10^5 10^7
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0



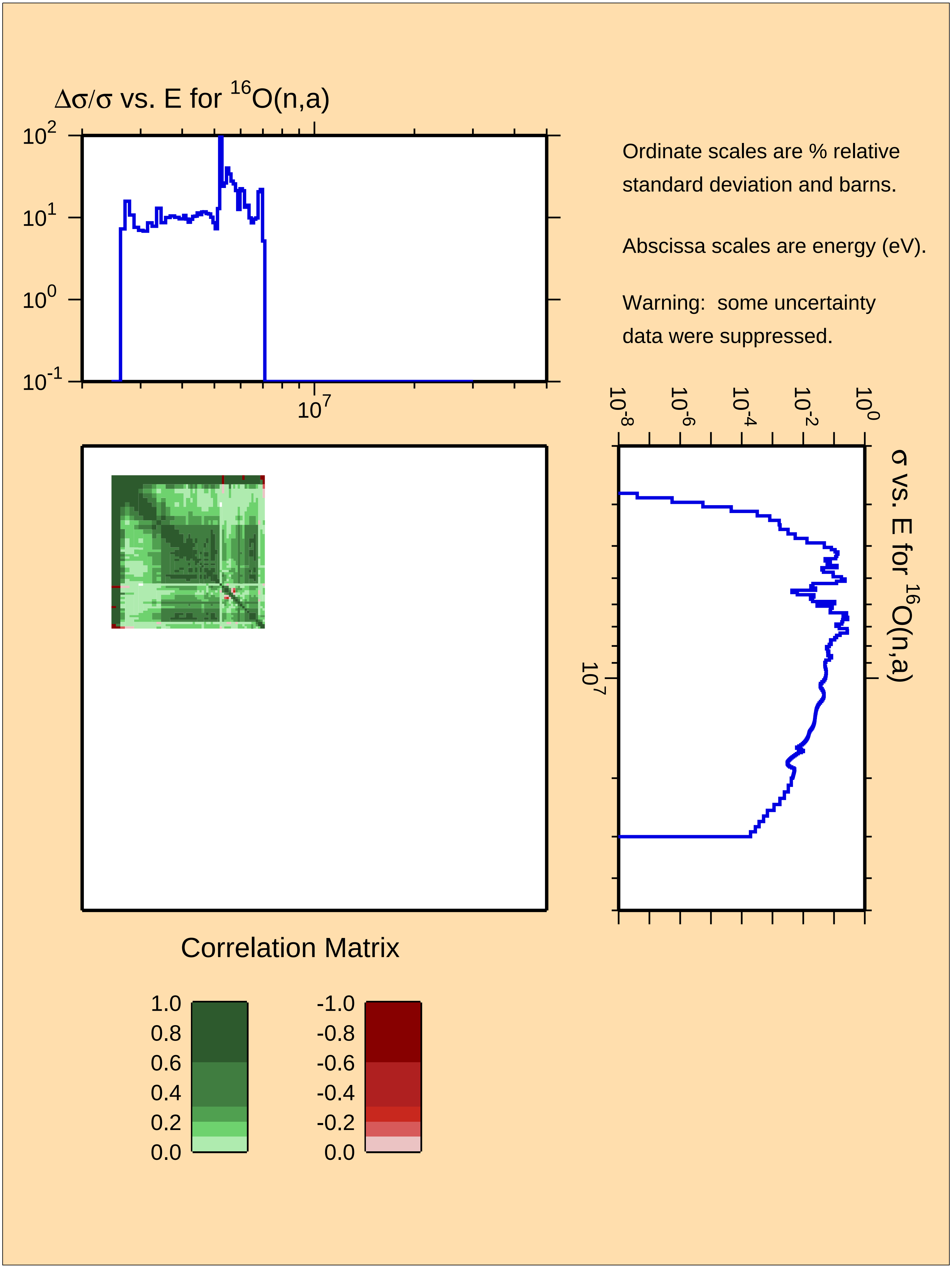
Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 12C(n,el.)
Δσ/σ vs. E for 12C(n,el.)
Correlation Matrix
1.0 0.8 0.6 0.4 0.2 0.0
-1.0 -0.8 -0.6 -0.4 -0.2 0.0



Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for $^{12}C(n,n_1)$
10^0
10^{-1}
10^{-2}
10^7
Δσ/σ vs. E for $^{12}C(n,n_1)$
16 14 12 10 8 6 4 2 0
10^7
Correlation Matrix
-1.0 -0.8 -0.6 -0.4 -0.2 0.0
1.0 0.8 0.6 0.4 0.2 0.0



Ordinate scales are % relative
standard deviation and barns.
Abscissa scales are energy (eV).
σ vs. E for 16O(n,el.)
10^2
10^1
10^0
10^-1
10^-3
10^-1
10^1
10^3
10^5
10^7
Δσ/σ vs. E for 16O(n,el.)
Correlation Matrix
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
1.0
0.8
0.6
0.4
0.2
0.0


Δσ/σ vs. E for 16O(n,a)
10^2
10^1
10^0
10^-1
10^7
Ordinate scales are % relative standard deviation and barns.
Abscissa scales are energy (eV).
Warning: some uncertainty data were suppressed.
σ vs. E for 16O(n,a)
10^-8
10^-6
10^-4
10^-2
10^0
10^7
Correlation Matrix
1.0
0.8
0.6
0.4
0.2
0.0
-1.0
-0.8
-0.6
-0.4
-0.2
0.0