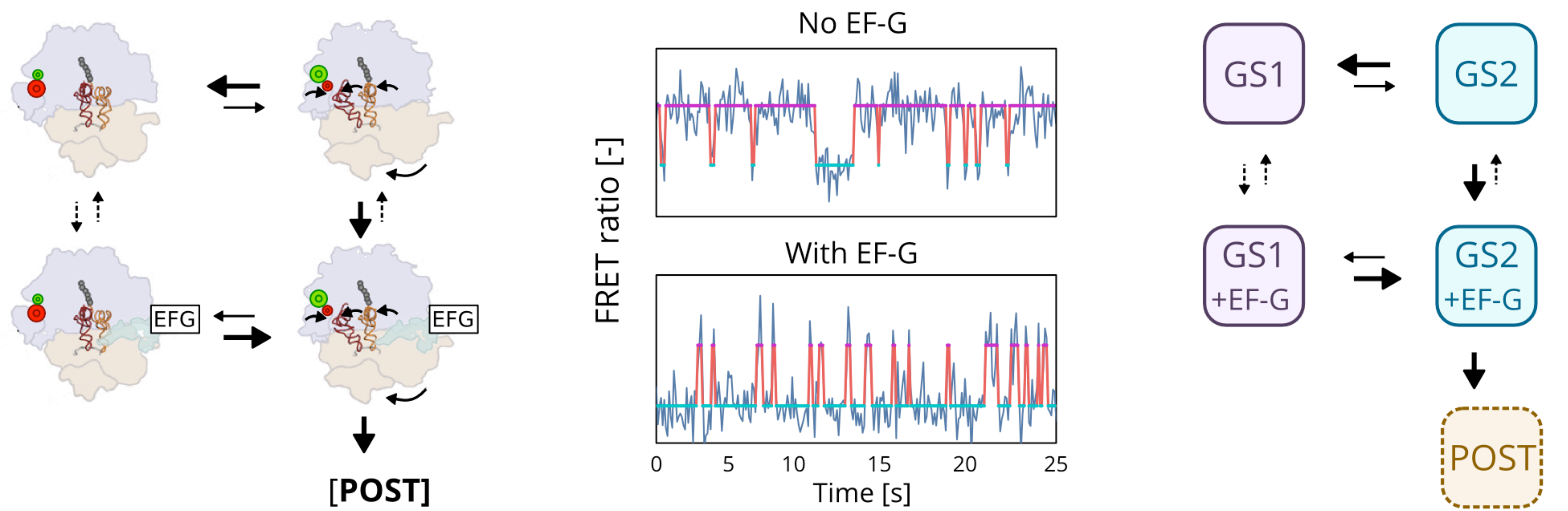
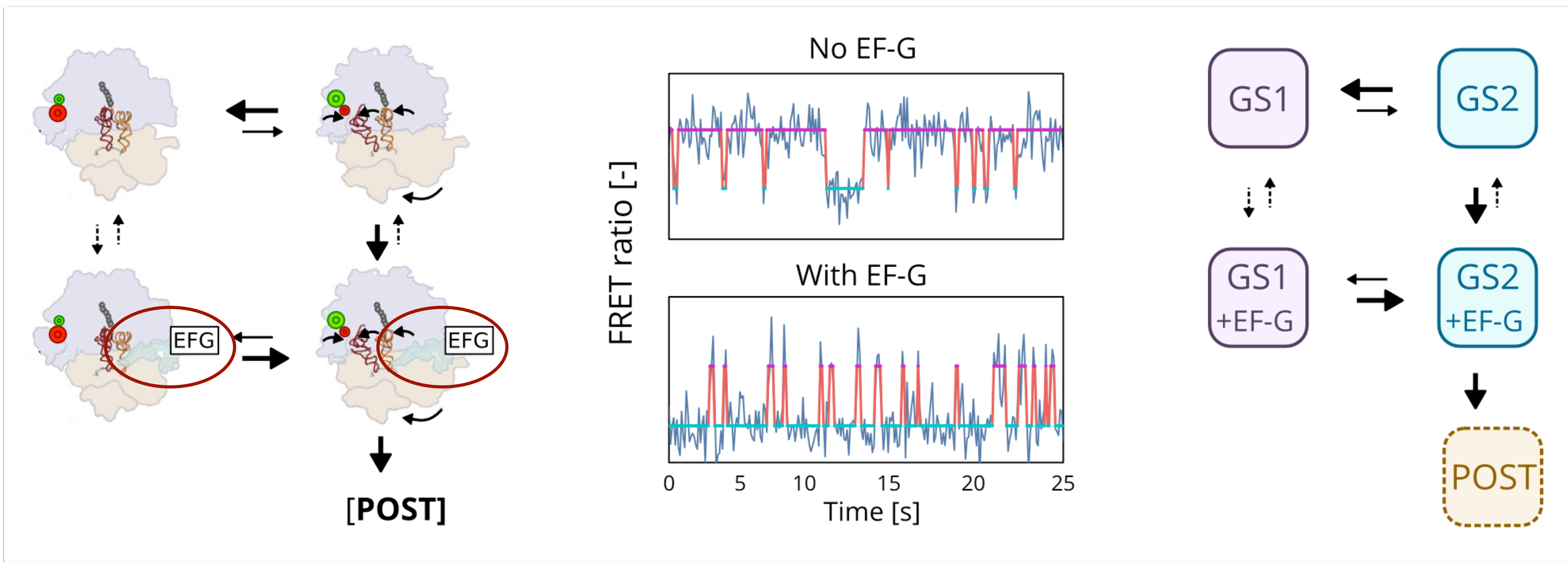
Learning Kinetic Models from Single-Molecule Experiments



Single-molecule FRET studies of the Ribosome

Ruben Gonzalez (Columbia)

Learning Kinetic Models from Single-Molecule Experiments



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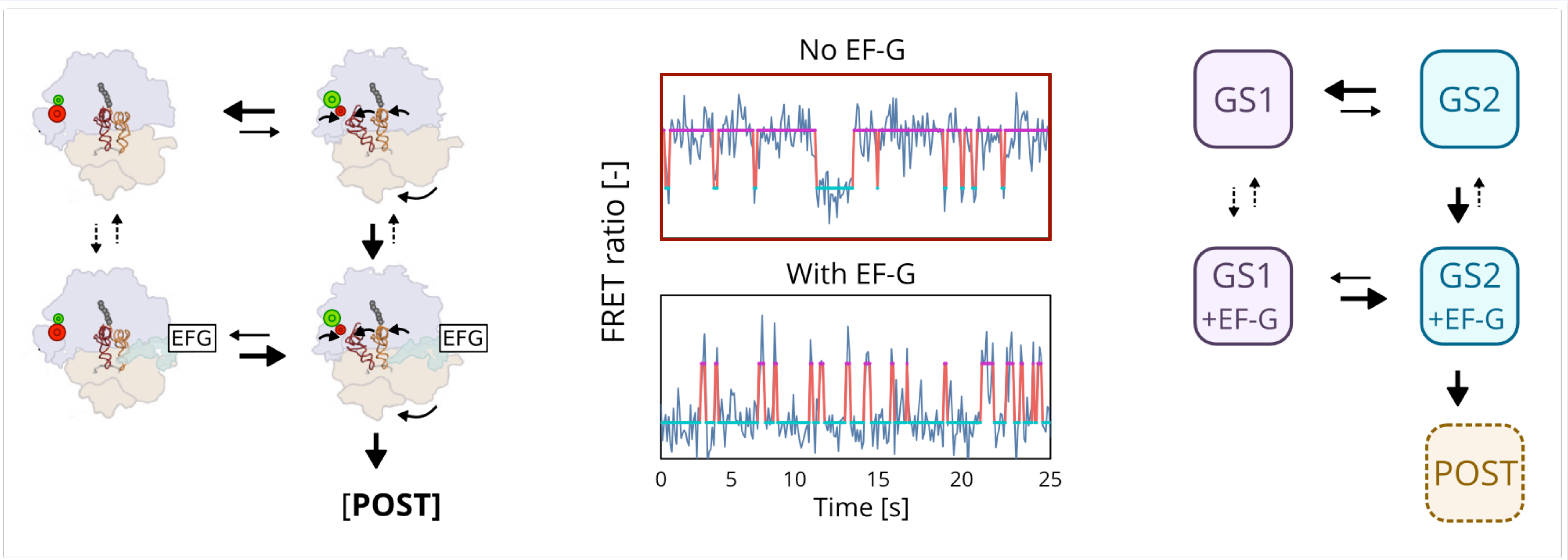

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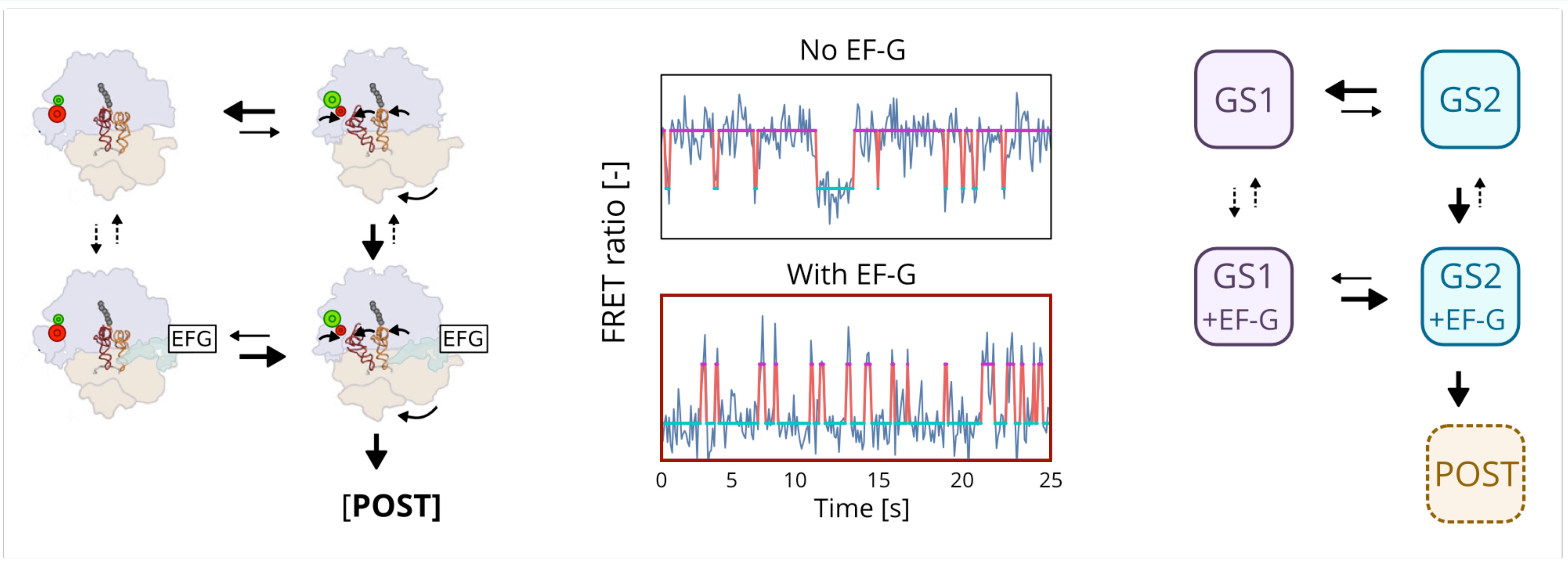

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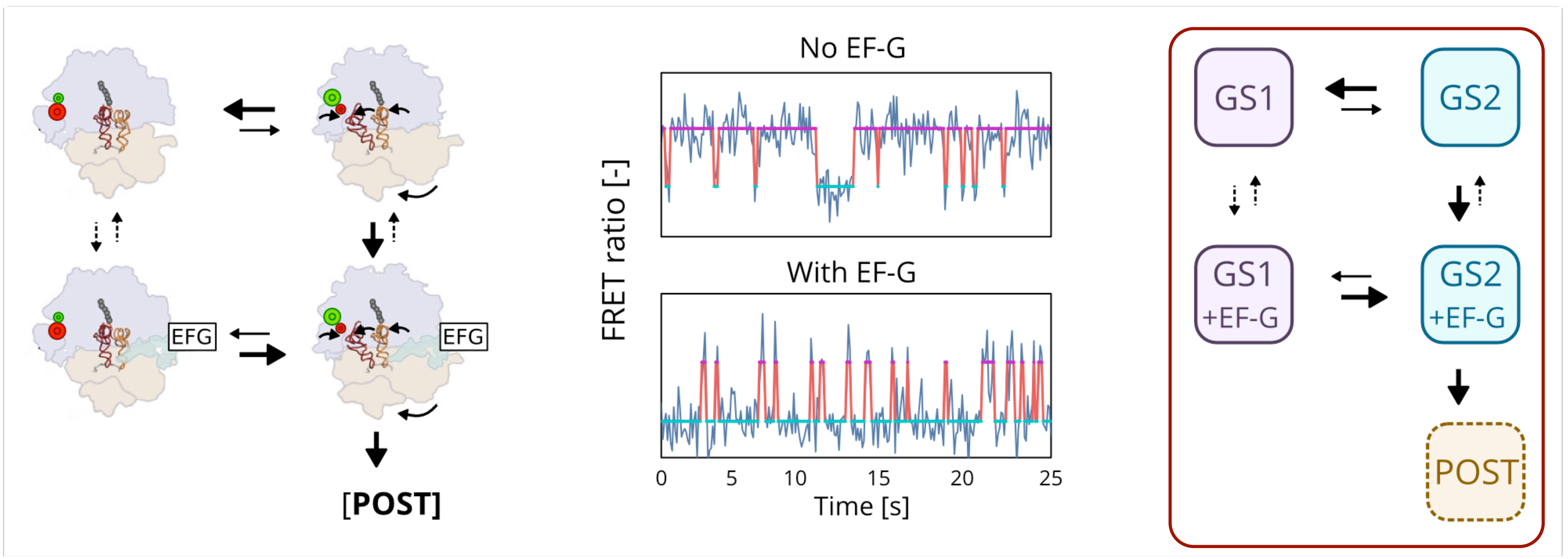

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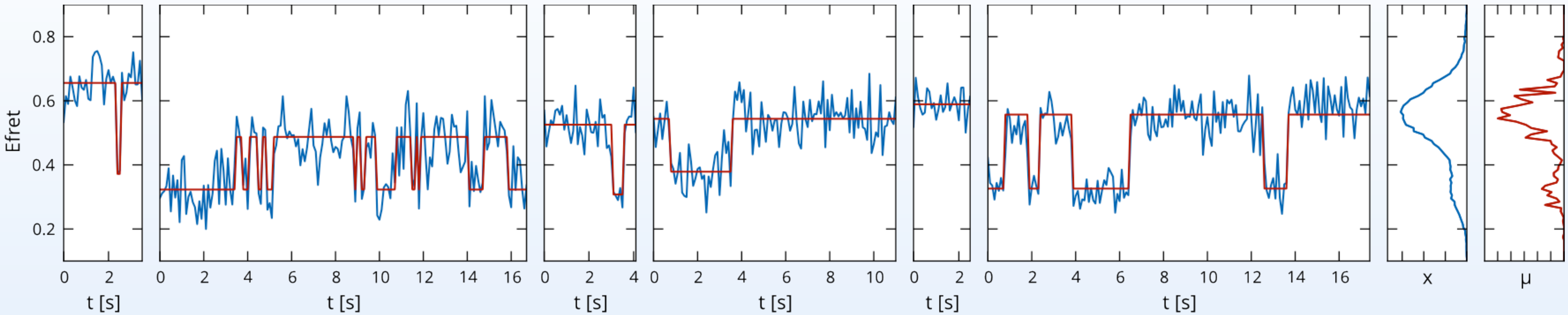
HMMs on multiple time series



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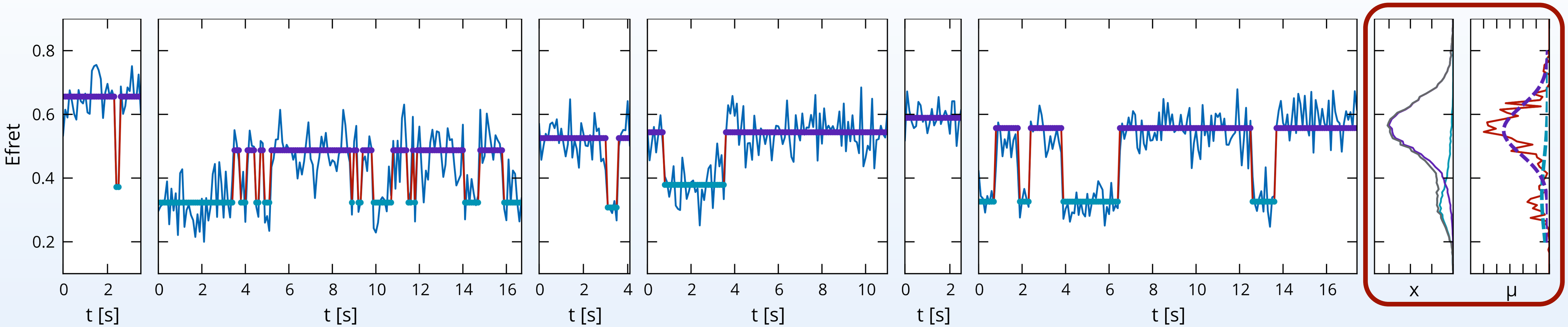
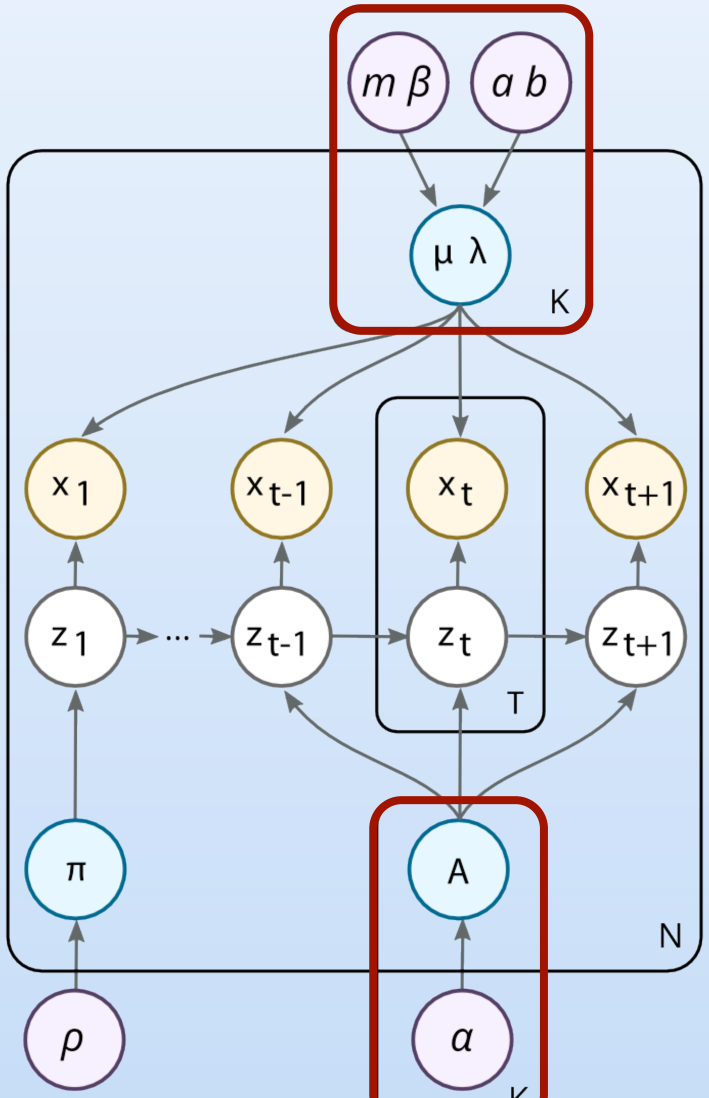
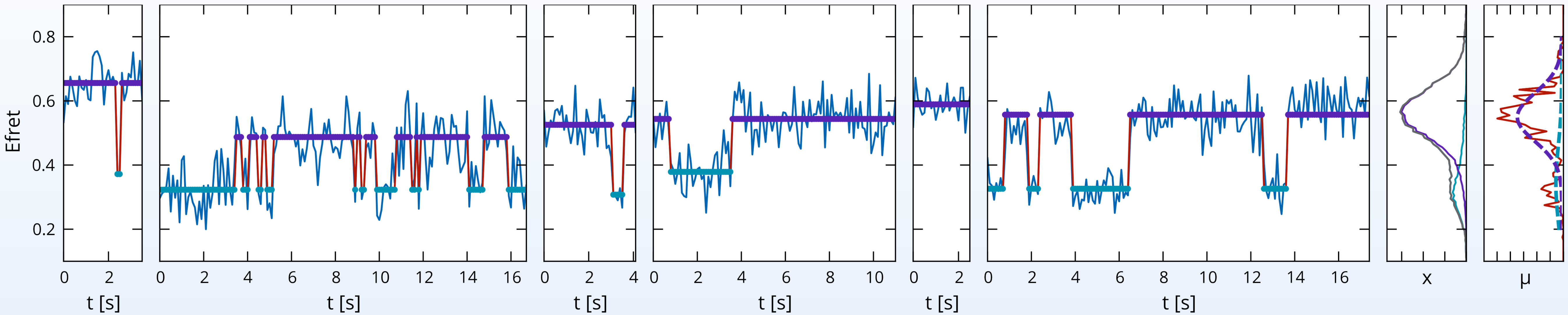




Hierarchical Coupling

$$\mu_{n,k} \sim \mathrm{Norm}(m_k, \beta_k \lambda_k)$$
$$\lambda_{n,k} \sim \mathrm{Gamma}(a_k, b_k)$$
$$A_{n,k} \sim \mathrm{Dir}(\alpha_k)$$
$$\pi_n \sim \mathrm{Dir}(\rho)$$

Hyperparameter Estimation



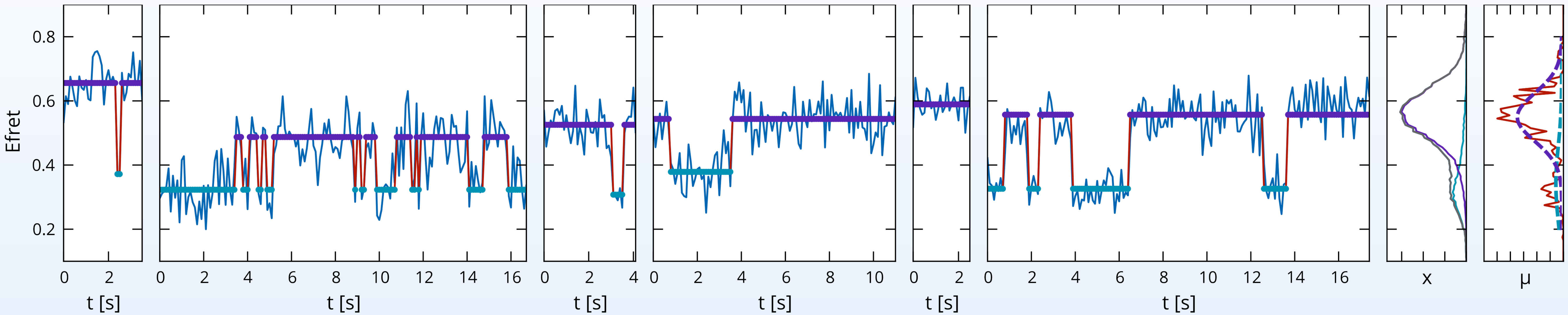
Variational Empirical Bayes

$$q(z_n) = \underset{q(z_n)}{\text{argmin}}\, D_{\text{KL}}[q(z_n)q(\theta_n) \,||\, p(z_n, \theta_n \,|\, x_n, \psi)]$$

$$q(\theta_n) = \underset{q(\theta_n)}{\text{argmin}}\, D_{\text{KL}}[q(z_n)q(\theta_n) \,||\, p(z_n, \theta_n \,|\, x_n, \psi)]$$

$$\psi = \underset{\psi}{\text{argmin}} \sum_n D_{\text{KL}}[q(\theta_n) \,||\, p(\theta_n \,|\, \psi)]$$

Hyperparameter Estimation



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$$q(z_n) = \underset{q(z_n)}{\operatorname{argmin}}\, D_{\mathrm{KL}}[q(z_n)q(\theta_n) \,\|\, p(z_n, \theta_n \mid x_n, \psi)]$$

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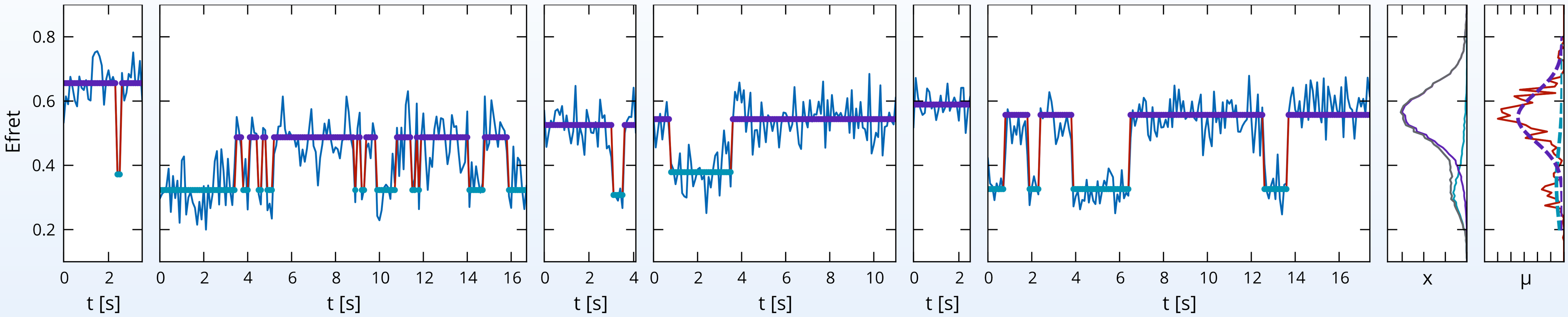

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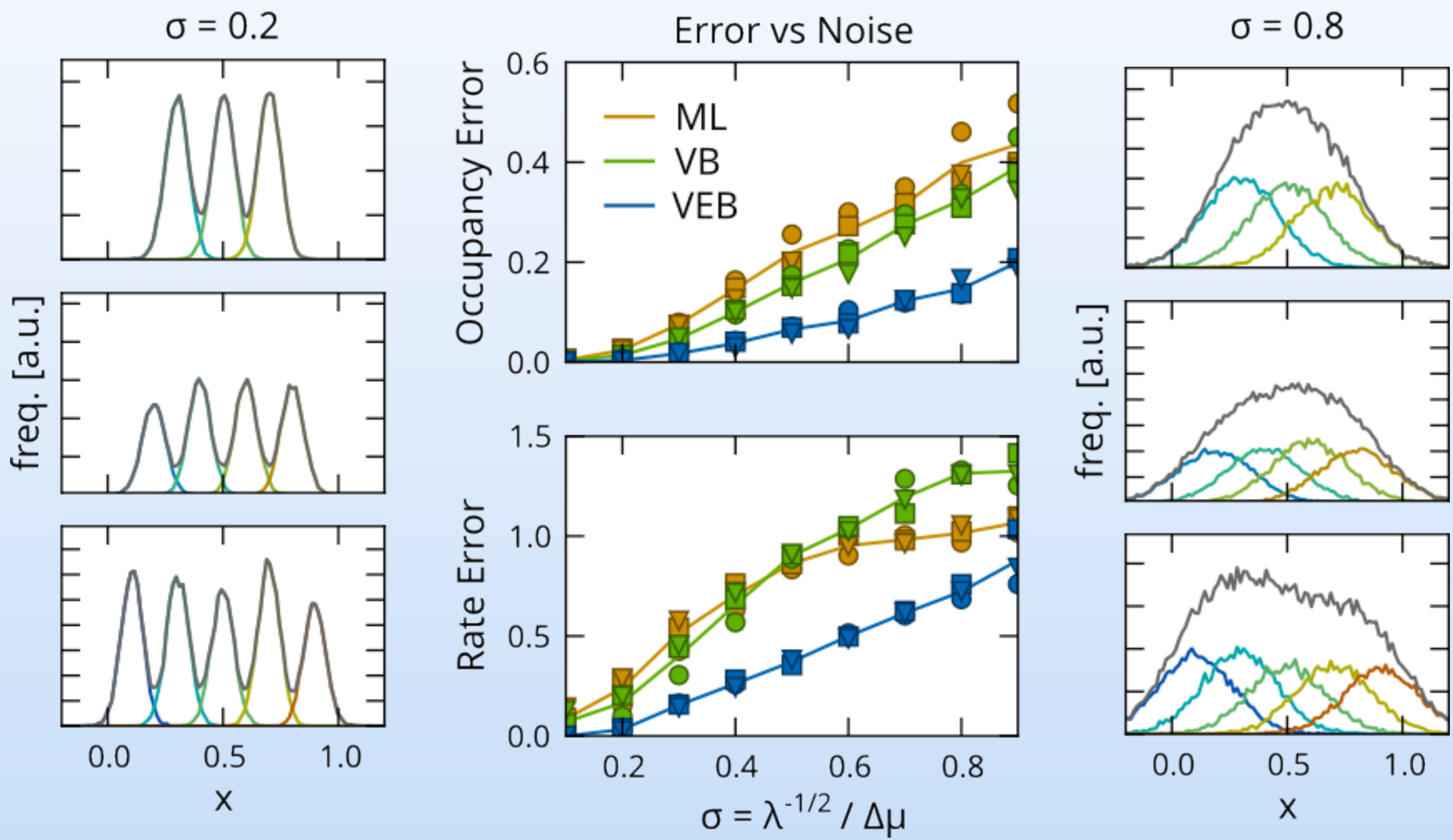
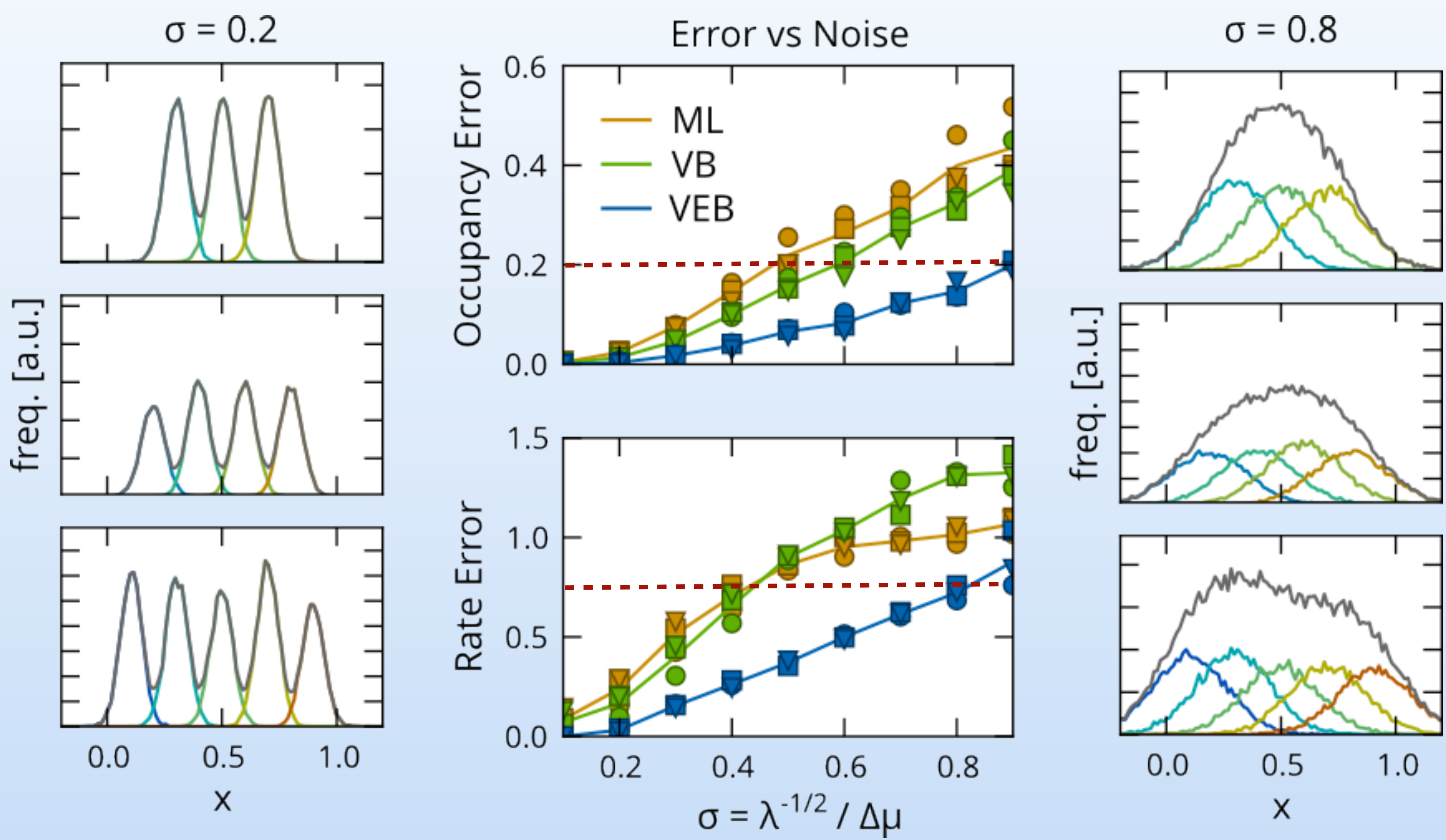
Transition Count Error vs Noise

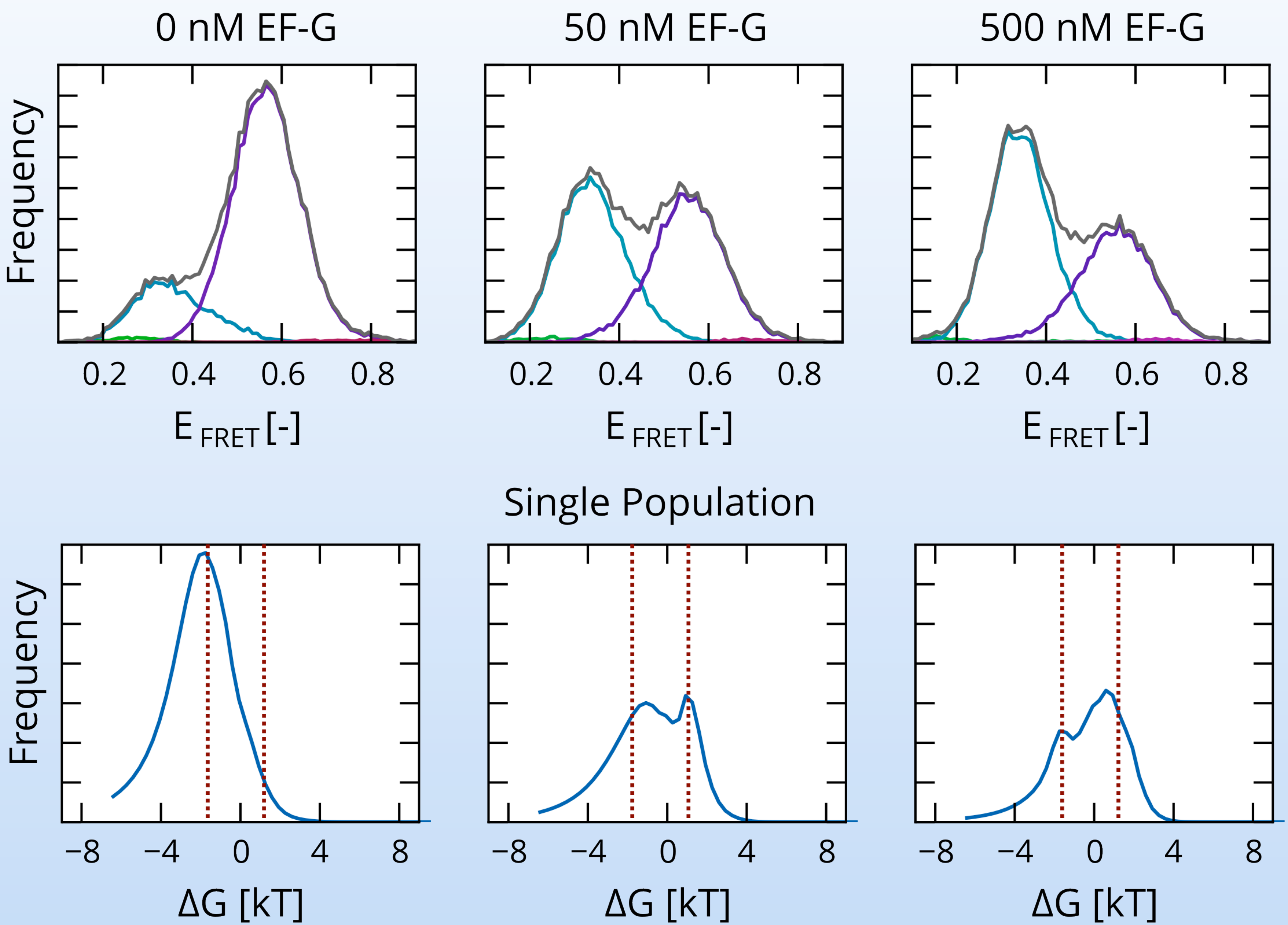


Transition Count Error vs Noise



Detecting Subpopulations

Fei, Bronson, Hofman, Srinivas, Wiggins, Gonzalez, PNAS, 2009



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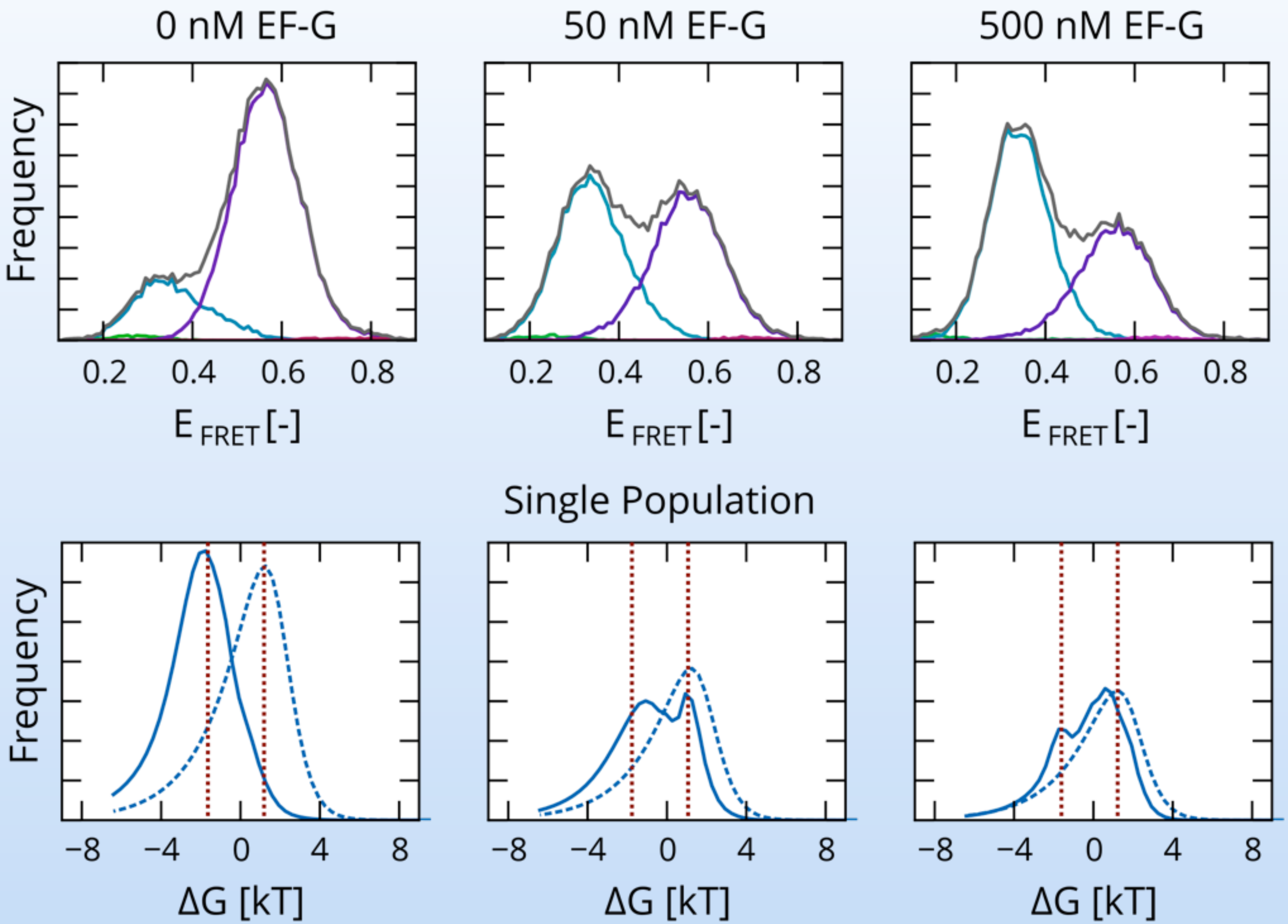

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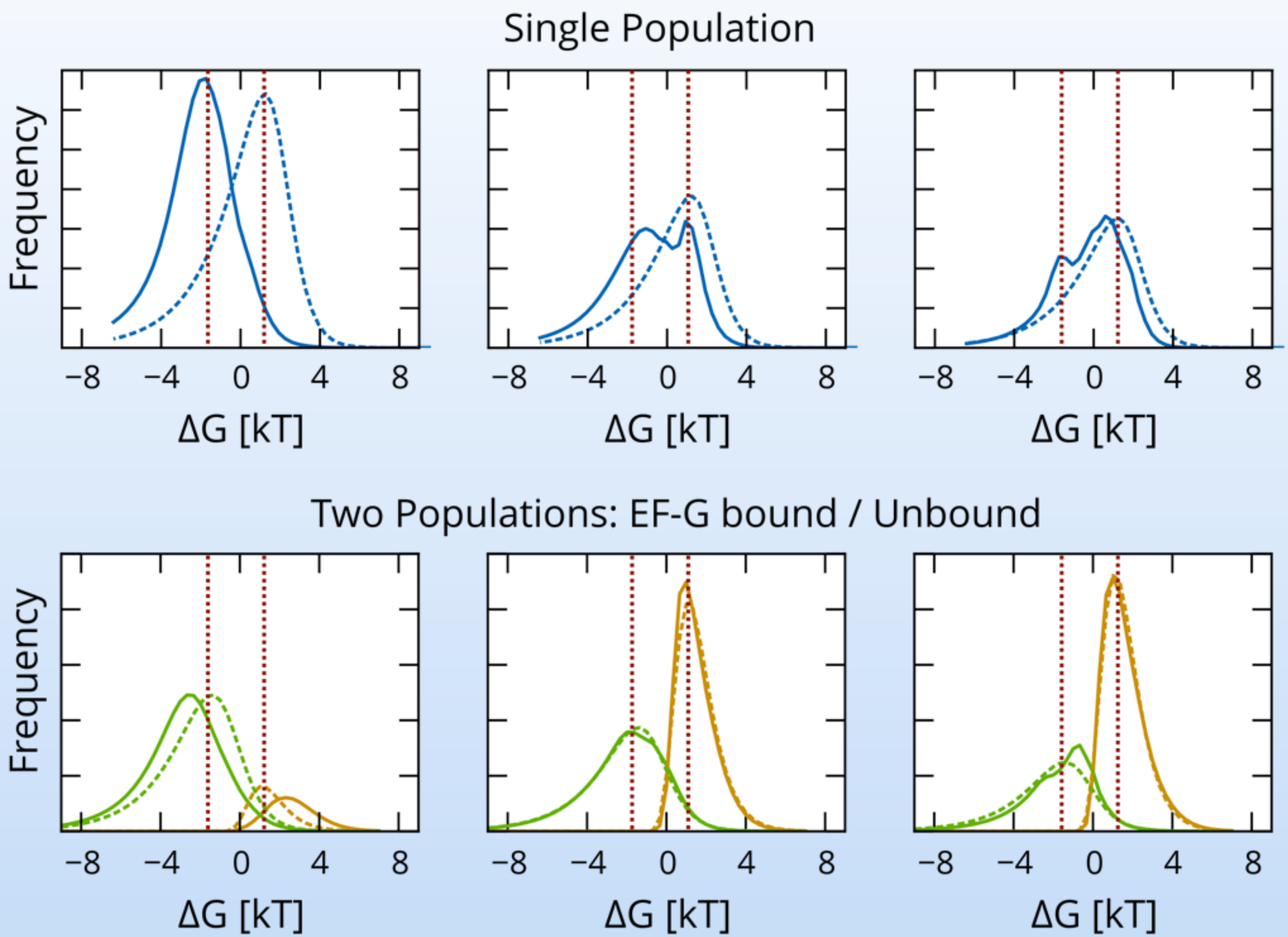

Co-conspirators

Columbia

Oxford

Jan-Willem
van de Meent

Chris
Wiggins

Ruben
Gonzalez

Frank
Wood

Poster 670

http://ebfret.github.io