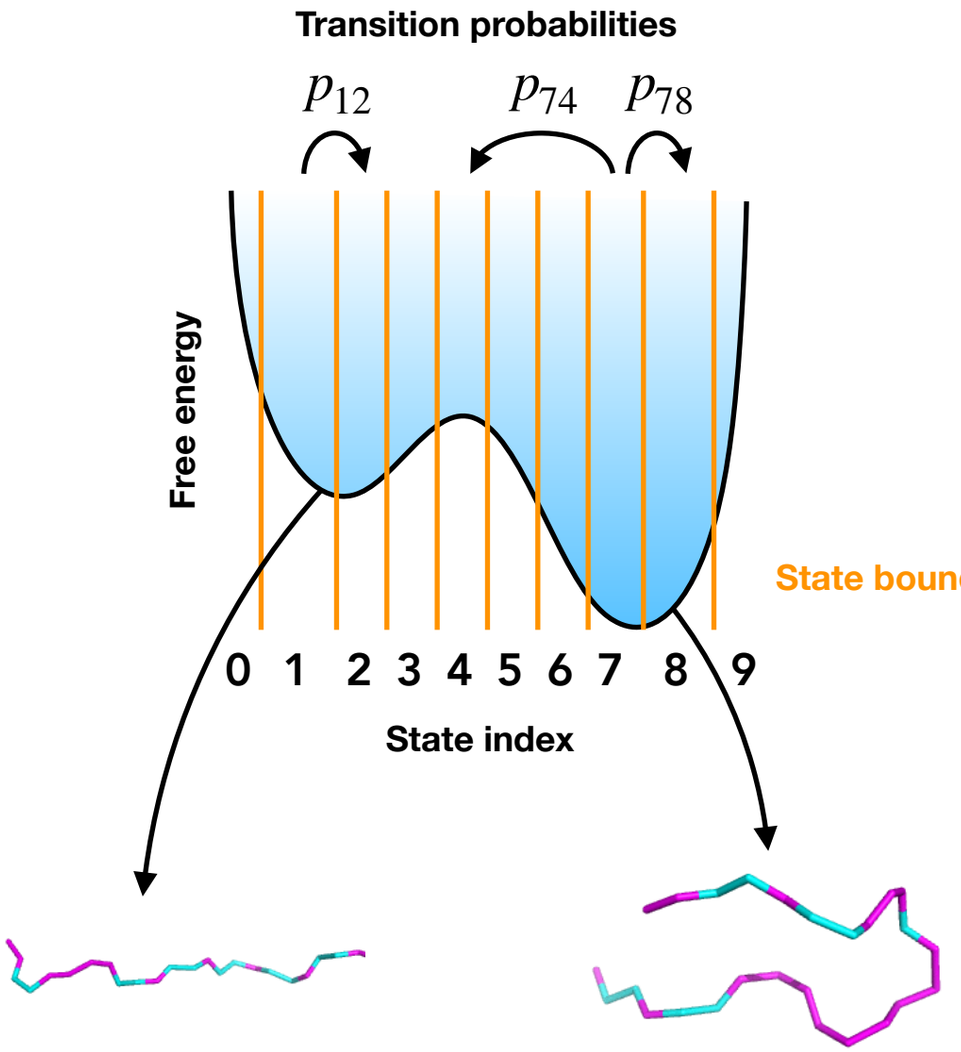
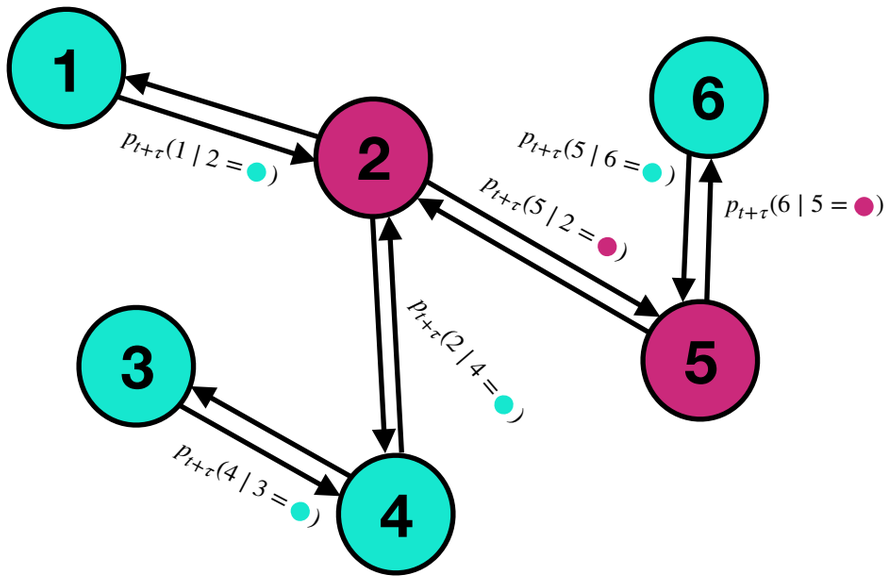


$\mathbf{s}_t = ($ ● , ● , ● , ● , ● , ● $)$



Markov state model

$$\mathbf{P}_\tau = \{\mathbb{P}(i \mid j, \tau)\} = \{p_{ij}\} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \cdots & & \cdots & \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{bmatrix}$$

Models exchange between
N mutually exclusive conformational states

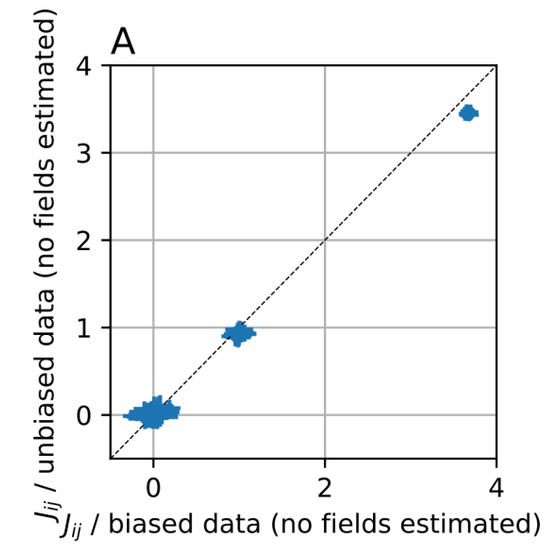
Markov random field

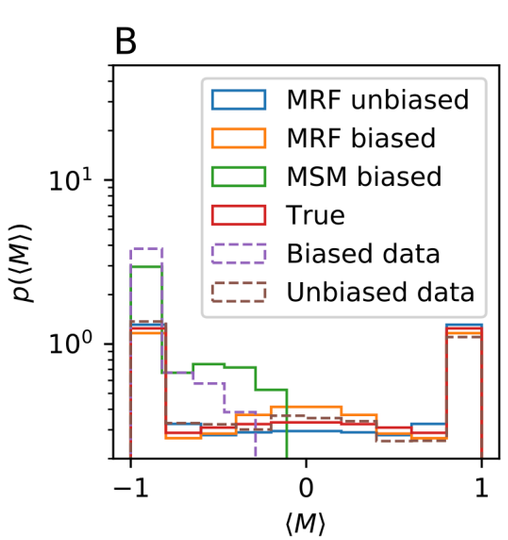
$$p(\mathbf{s}_{t+\tau} \mid \mathbf{s}_t) = \prod_i^M p(s_{t,i} \mid \mathbf{s}_t)$$

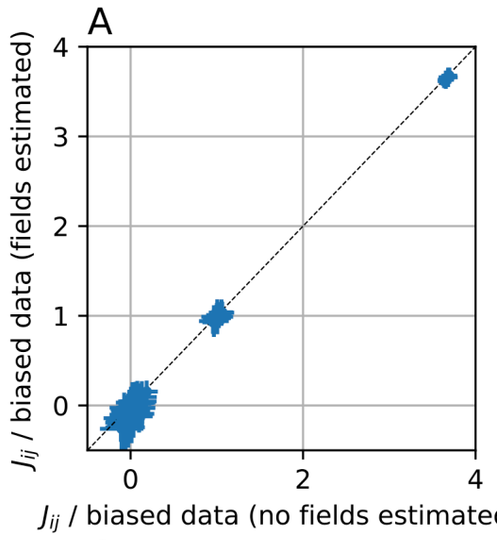
$$= \prod_i^M \frac{\exp[h_i^l + \sum_j^M \sum_k^{Q_i - 1} J_{i,j}^{l,k} - 2J_{i,j}^{l,k} \mathcal{I}_k(s_{t,j})]}{1 + \sum_m^{M-1} \exp[h_i^m + \sum_j^M \sum_k^{Q_m - 1} J_{i,j}^{m,k} - 2J_{i,j}^{m,k} \mathcal{I}_k(s_{t,j})]}$$

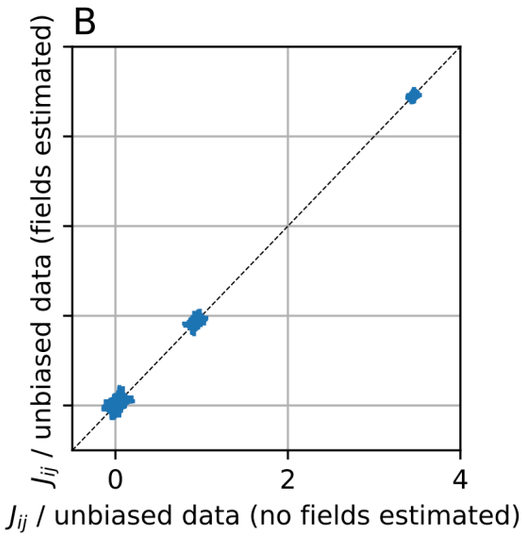
Models dynamics of
M sub-systems, i each with Q_i states.

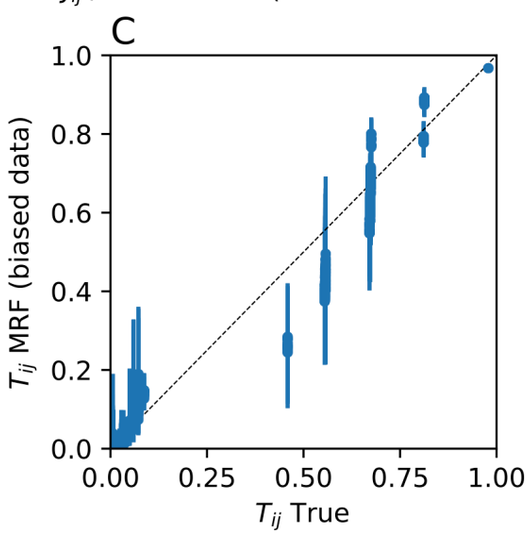
Inverse inference of Glauber dynamics on 9 spin Ising model with data on only one meta-stable state

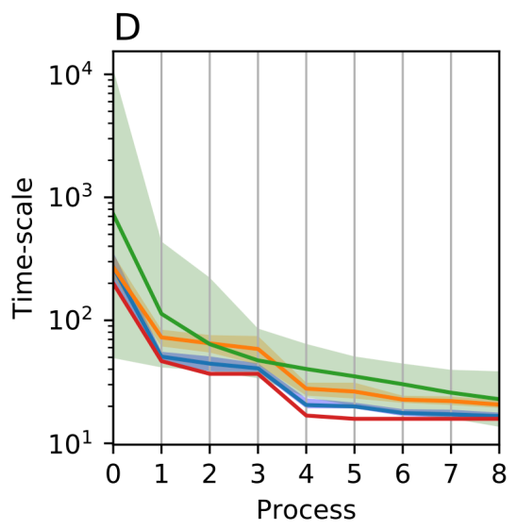


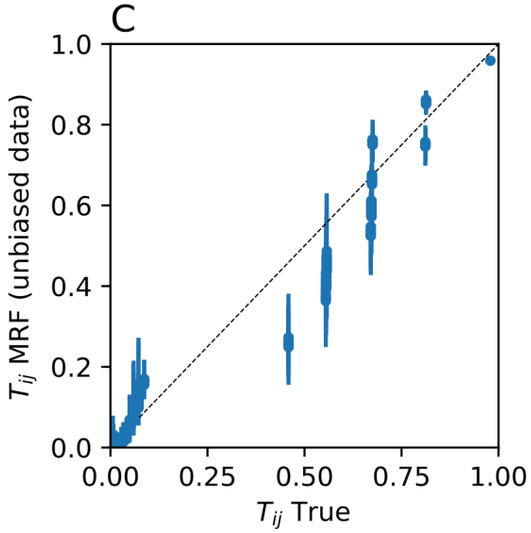


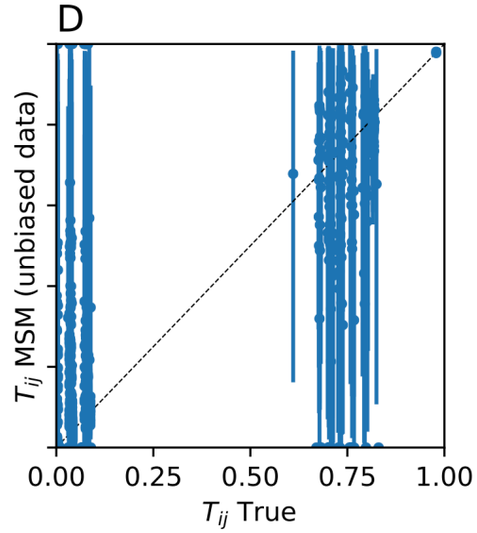






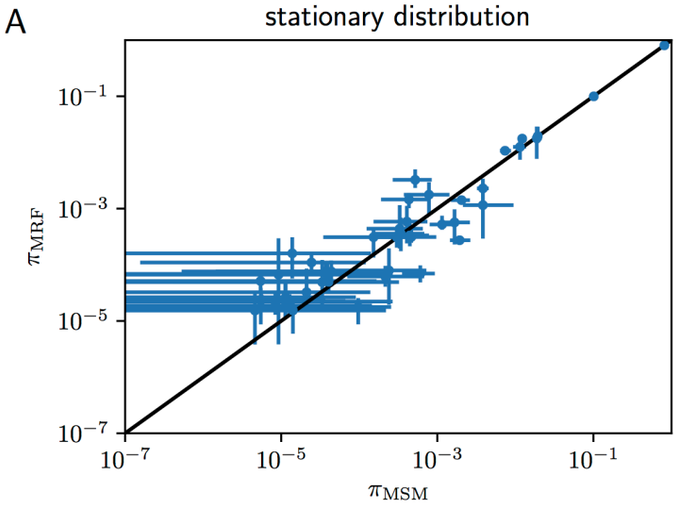




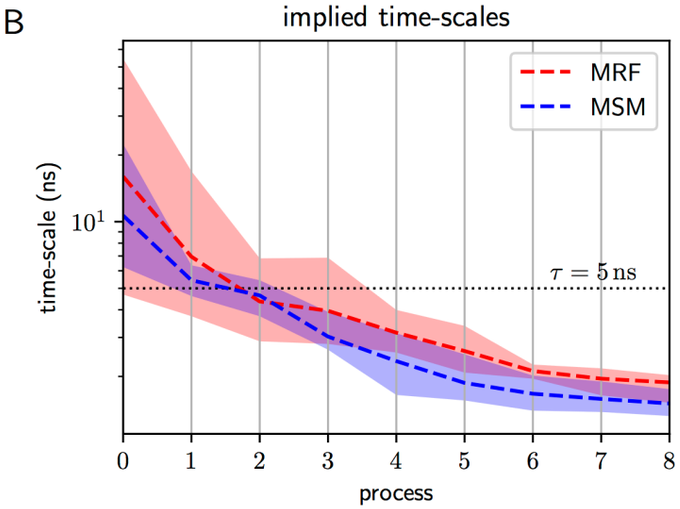


MRF of penta-peptide back-bone torsion rotamer dynamics

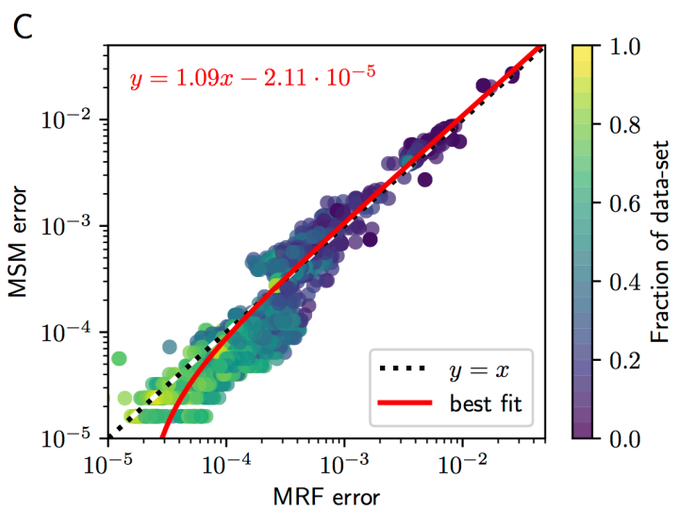
A



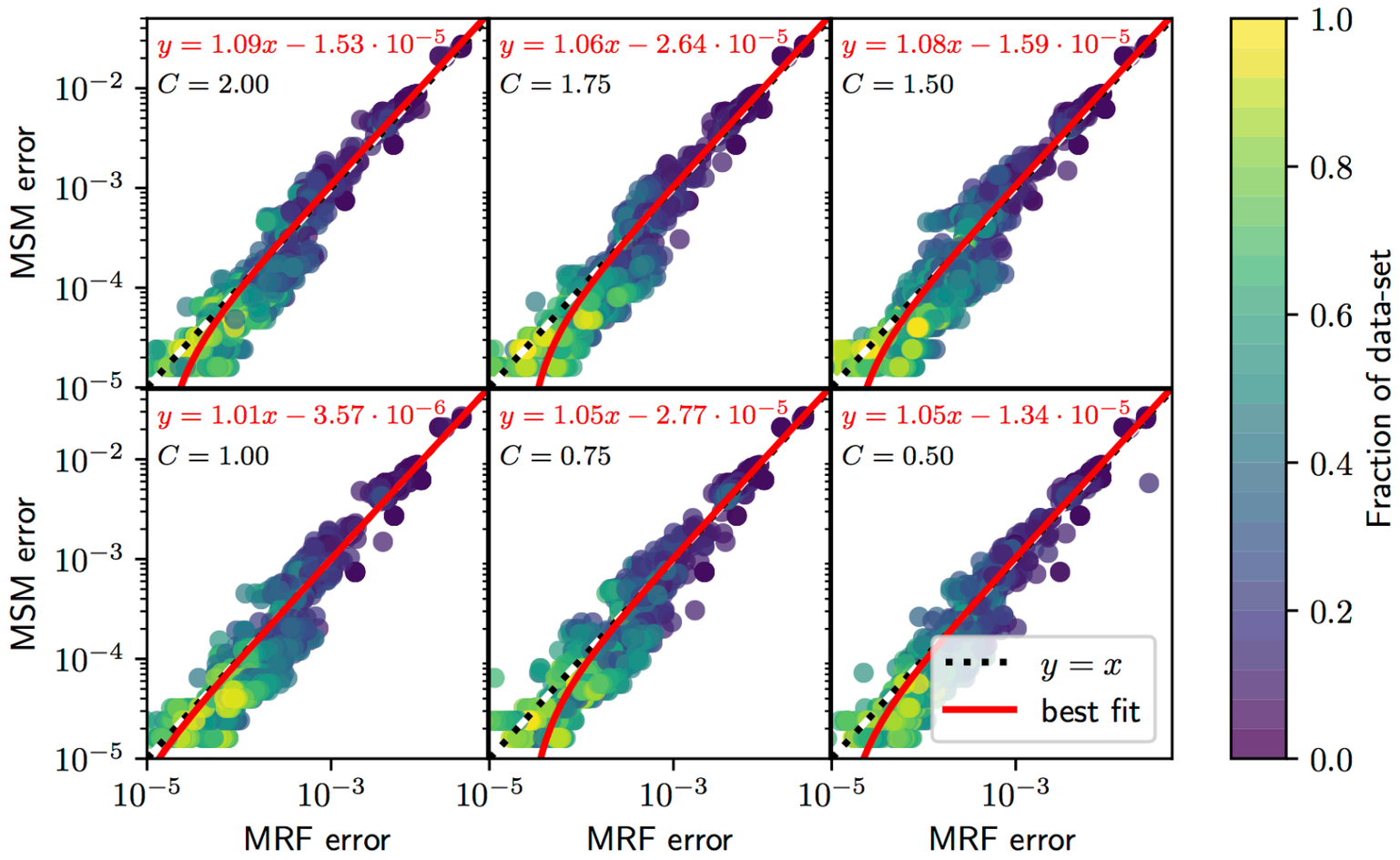
B



C

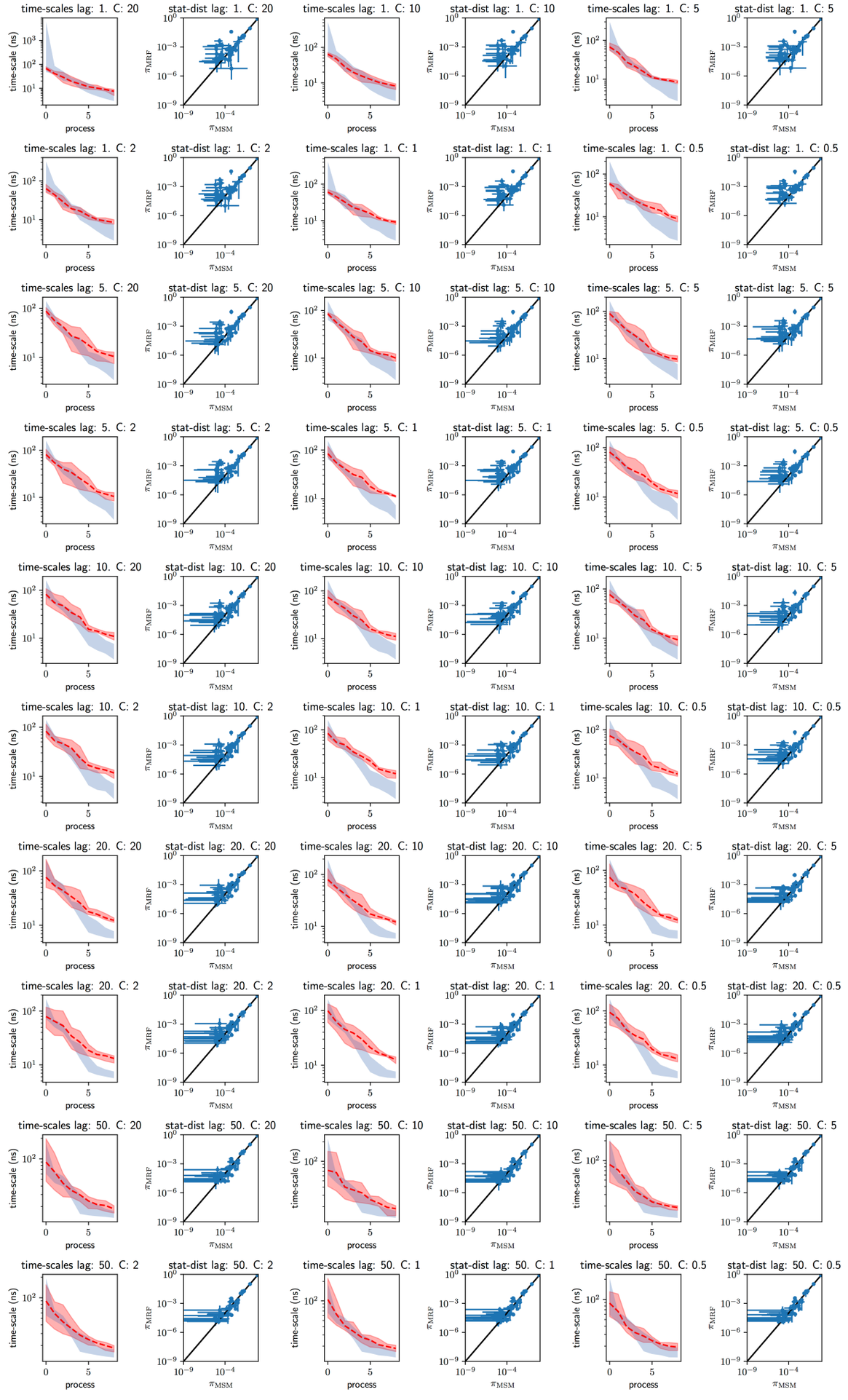


Prediction-error of unseen Markov states



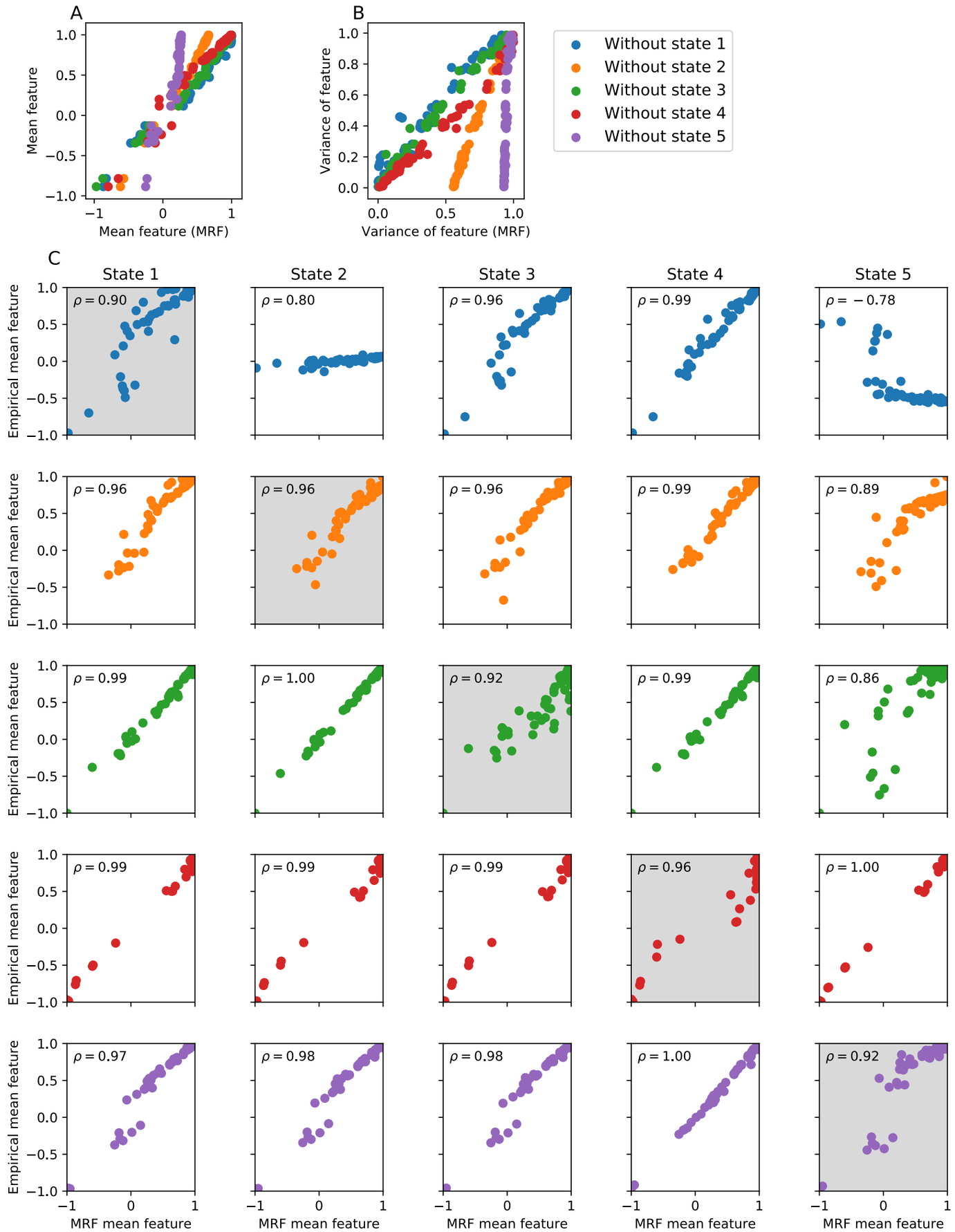
MRF of penta-peptide back-bone torsion rotamer dynamics

Stationary and dynamic parameters as a function of regularization parameters



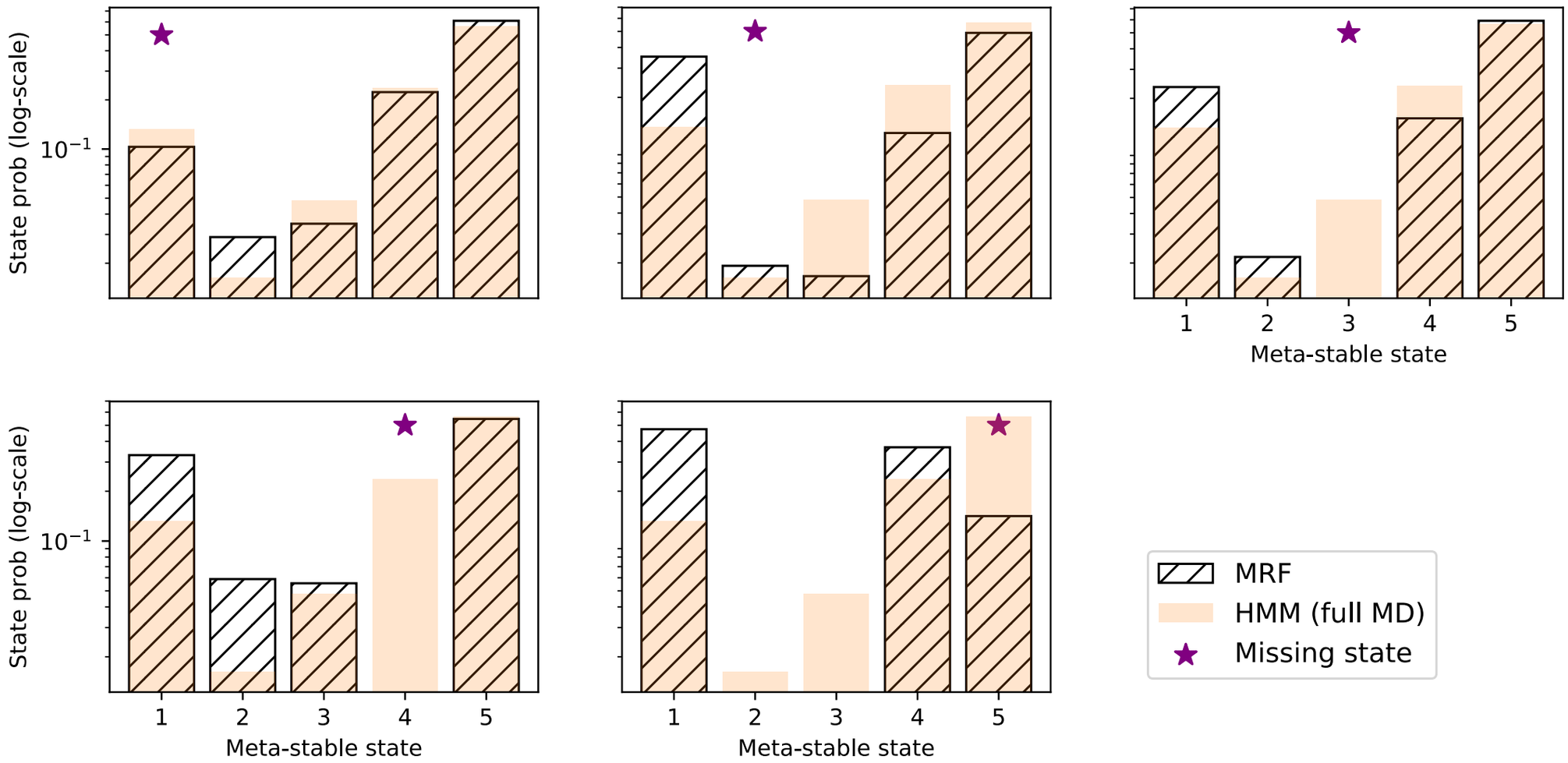
Villin Dihedral rotamer MRF

Prediction of global mean (A) and variance(B), of state-vectors when certain meta-stable states are unseen. Prediction of state vectors in reduced data sets (C)



Villin Dihedral rotamer MRF

Prediction of meta-stable state distributions without the different states



Villin Dihedral rotamer MRF

TICA projections