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Multisequence algorithm for coarse-grained biomolecular simulations: Exploring the sequence-structure relationship of proteins

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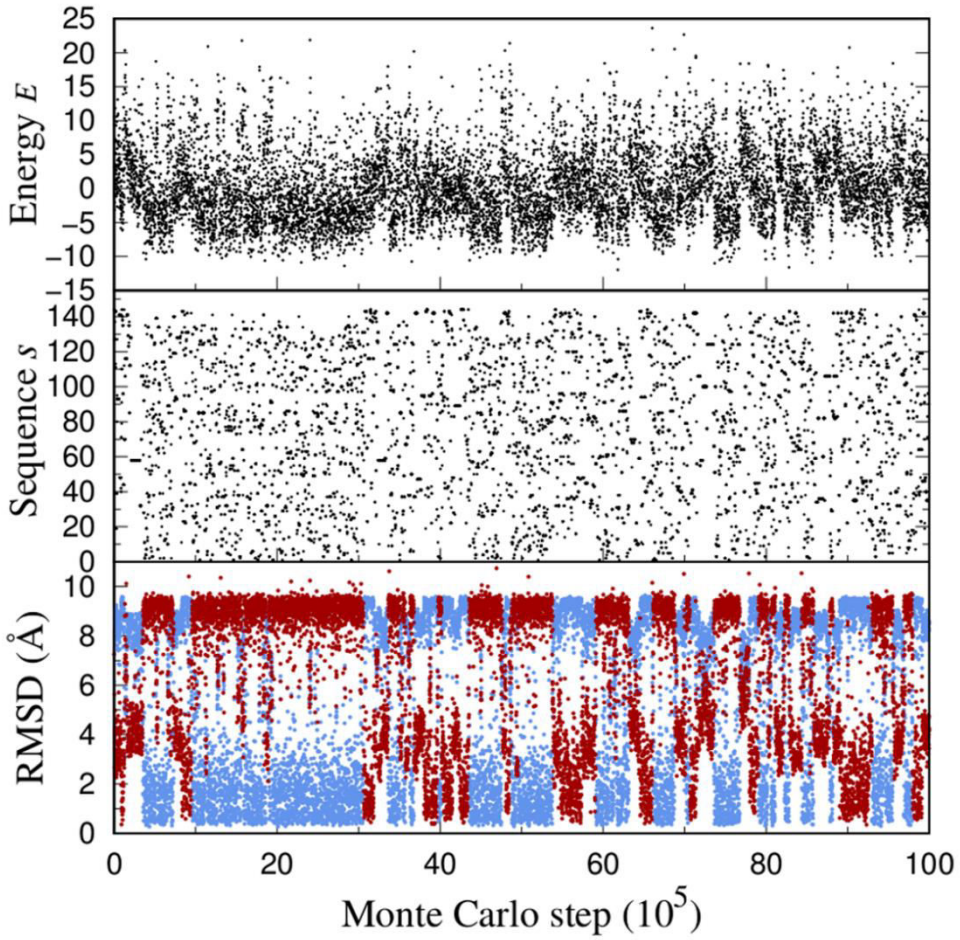
MULTISEQUENCE ALGORITHM FOR COARSE-GRAINED BIOMOLECULAR SIMULATIONS: EXPLORING THE SEQUENCE-STRUCTURE RELATIONSHIP OF PROTEINS

- We consider a multisequence (MS) algorithm for simulations of biomolecules.
- The MS algorithm provides the thermodynamic data to systematically investigate how proteins switch folds.
- Our model proteins exhibit reduced stability near the switch point.
- Bistable sequences are relatively less stable but play a crucial role in bridging two different folds.

A



Example of a multisequence simulation

B

Fold IA

C

Fold IB