Novel, provable algorithms for efficient ensemble-based computational protein design and their application to the redesign of the c-Raf-RBD:KRas protein-protein interface (Supporting information)

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S4 Text. Sequence and partition function approximation algorithms.

K^* is a partition function approximation algorithm that approximates a single partition function q_{pl}, q_p, or q_l for a single sequence [1–3]. Historically we have overloaded the term K^* to refer to both the partition function approximation algorithm and the ratio of partition functions: $q_{pl}/q_p q_l$. The *BBK** algorithm implements a search strategy over sequence space to find the best sequences ranked by this score. In doing so, *BBK** calls the K^* partition function approximation algorithm as a subroutine. In contrast, in the new work herein, *EWAK** is designed as a replacement for the K^* partition function approximation algorithm. Therefore, we compared *BBK** with K^* to *BBK** with *EWAK** for testing purposes.

FRIES is effectively a preprocessing algorithm that is agnostic to the method of partition function calculation, and therefore is run before *BBK**.

References

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