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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S1 Text. Homology model of c-Raf-RBD in complex with KRas

PDB ID 4DSN [1] is an X-ray crystal structure of KRas isoform 2B which contains G12D, a mutation that locks KRas into its active form. This structure of KRas bound to a GTP analog was used to model KRas^{GTP}. PDB ID 1GUA [2] is an X-ray crystal structure of c-Raf in complex with Rap, a Ras homolog. These two structures (4DSN and 1GUA) were aligned using PyMol [3]. Rap was then removed, leaving c-Raf poised in complex with KRas from PDB ID 4DSN. This complex was then minimized using Sander from AmberTools for 200 steps [4] to relax any steric clashes.

References

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