

Supporting Information

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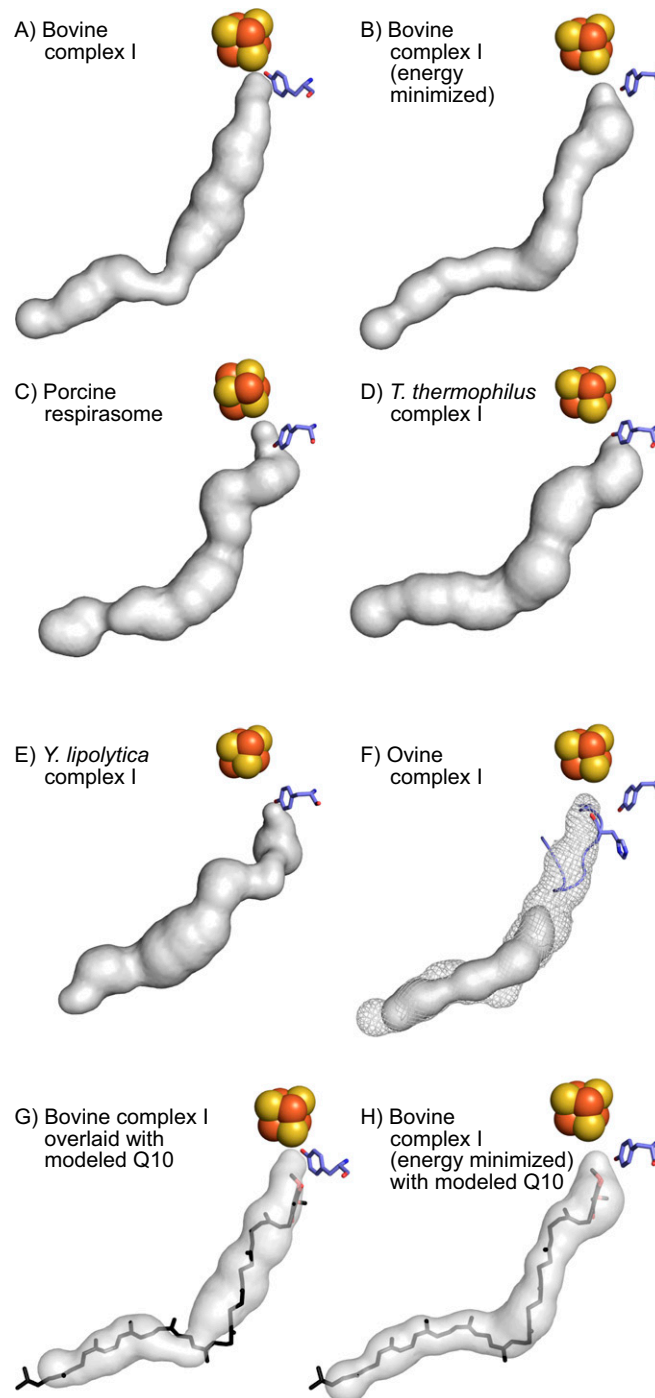


Fig. S1. Predicted quinone-binding cavities in published complex I structures. (A) The active state of bovine complex I (PDB ID: 5LC5) (6). (B) The bovine structure with Q10 modeled in using MD simulations (Q10 was removed for the channel prediction). (C) Complex I from the porcine respirasome (PDB ID: 5GUP) (7). (D) *T. thermophilus* complex I (PDB ID: 4HEA) (10). (E) *Y. lipolytica* complex I (PDB ID: 4WZ7) (9). (F) Ovine complex I (PDB ID: 5LNK) (8) in which the cavity is blocked by the $\beta 1$ - $\beta 2^{49}$ kDa loop; the cavity from A is overlaid as a mesh for comparison. (G) The active state of bovine complex I (PDB ID: 5LC5) with the modeled Q10 structure overlaid. (H) The bovine structure with Q10 modeled in using MD simulations. Cluster N2 is shown as spheres and Y108^{49kDa} is shown because its hydroxyl oxygen was used as the starting point for cavity searches. Channels were predicted using the Caver 3.0 plugin in PyMOL (33) with a probe size of 1.4 Å or 1.1 Å for E.

