A trick of the tail: computing the entropic contribution to the energetics of quinone-protein unbinding

Supporting information

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Figure S1. Entropic contributions to the free energy as a function of the isoprenoid side chain length. Linear regression analysis of the data presented in table 1 of the main article. Bullet symbols: computed data, solid line: linear regression line, dashed line: theoretical limit for an acceptance ratio of unity in eq. 1, main article. This corresponds to a fully flexible chain with 18 dihedral angle states per isoprene monomer.
Figure S2. Level plot of the menaquinol dihedral angles, with letters as indicated in figure 1 of the main article. Black: MHK4, green: MHK6, red: MHK8.
Figure S3. Number of unique conformations found during the MD simulation as a function of time. The lines represent menaquinol-6 (orange dashed line) and menaquinone-6 (full orange line) in n-hexane. In addition, we show menaquinol-8 (red dashed line), menaquinone-8 (full red line), menaquinol-6 (green dashed line) menaquinone-6 (full green line), menaquinol-4 (blue dashed line) menaquinone-4 (full blue line), all embedded in a lipid bilayer membrane.
Dihedral angles

Angles are enumerated according to their position in the side chain with reference to the naphtoquinone moiety of the quinone or quinol, cf. figure 1 of the main article.

We have:

- angles 3, 6, 9, ... = $\phi_{badc}$
- angles 4, 7, 10, ... = $\phi_{adcb}$
- angles 5, 8, 11, ... = $\phi_{dcba}$
Figure set S4. Menaquinol-4 (MHK4) in a lipid bilayer
Figure set S5. Menaquinol-6 (MHK6) in a lipid bilayer
10

angle 1

Counts

dihedral angle/
degrees

angle 2

Counts

dihedral angle/
degrees

angle 3

Counts

dihedral angle/
degrees

angle 4

Counts

dihedral angle/
degrees

angle 5

Counts

dihedral angle/
degrees

angle 6

Counts

dihedral angle/
degrees

angle 7

Counts

dihedral angle/
degrees

angle 8

Counts

dihedral angle/
degrees
Figure set S6. Menaquinol-6 (MHK6) in n-hexane
Figure set S7. Menaquinol-8 (MHK8) in a lipid bilayer
Figure set S8. Menaquinone-4 (MK4) in a lipid bilayer
Figure set S9. Menaquinone-6 (MQ6) in n-hexane
Figure set S10. Menaquinone-6 (MQ6) in a lipid bilayer
Figure set S11. Menaquinone-8 (MQ8) in a lipid bilayer
The image contains six histograms, each labeled with a different angle (angle 9 to angle 16). Each histogram plots the counts of dihedral angles in degrees. The x-axis represents the dihedral angle in degrees, ranging from 0 to 360, while the y-axis represents the counts.