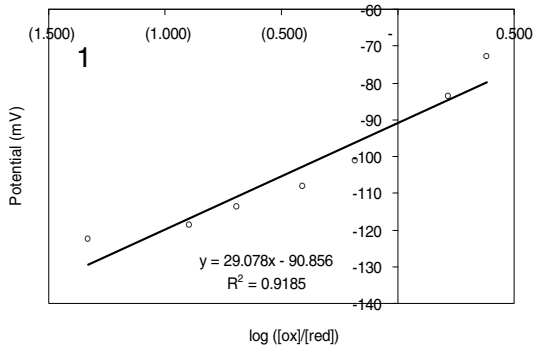
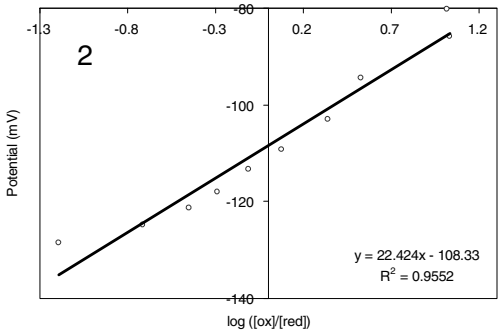
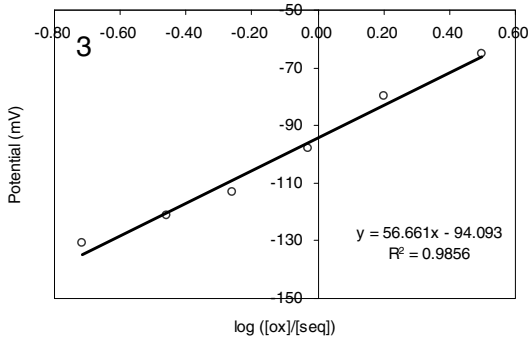
Supporting Information for

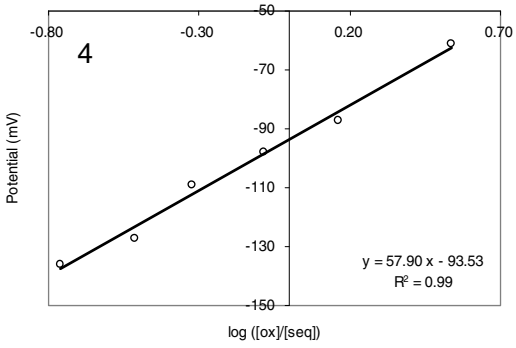
A hydrogen-bonding network is important for oxidation and isomerization in the reaction catalyzed by cholesterol oxidase

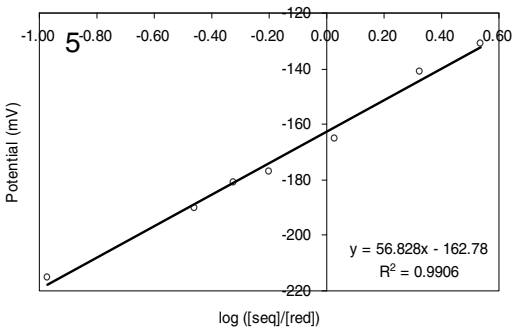
Artem Y. Lyubimov, Lin Chen, Nicole S. Sampson, and Alice Vrielink

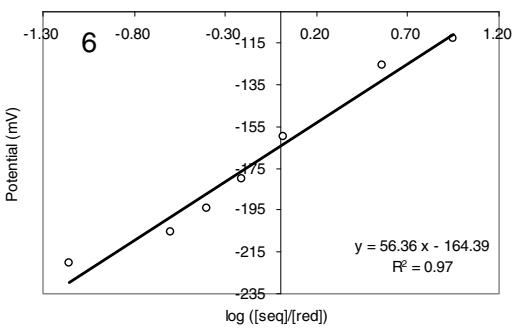

1
Potential (mV)
log ([ox]/[red])
y = 29.078x - 90.856
R² = 0.9185

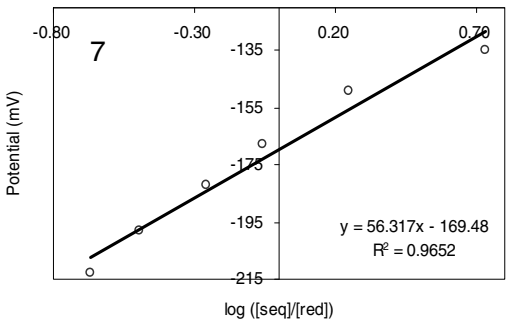

2
Potential (mV)
log ([ox]/[red])
y = 22.424x - 108.33
R² = 0.9552

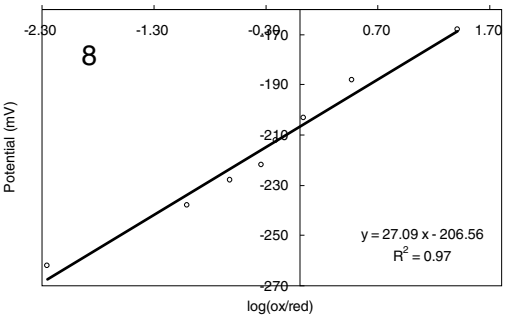

3
Potential (mV)
log ([ox]/[seq])
y = 56.661x - 94.093
R² = 0.9856

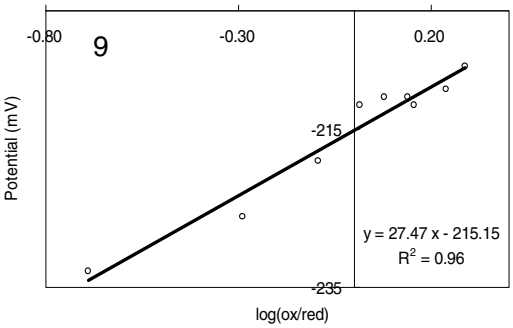

4
Potential (mV)
log ([ox]/[seq])
y = 57.90 x - 93.53
R² = 0.99

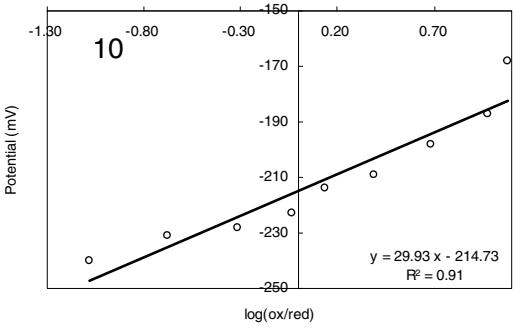

5
Potential (mV)
log ([seq]/[red])
y = 56.828x - 162.78
R² = 0.9906

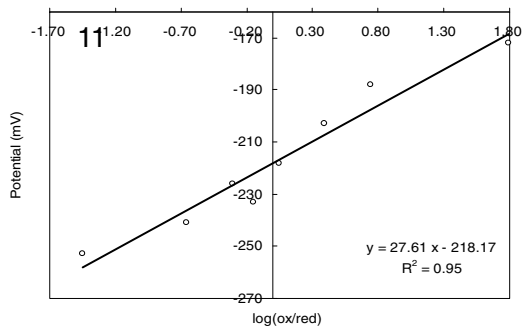

6
Potential (mV)
log ([seq]/[red])
y = 56.36 x - 164.39
R² = 0.97

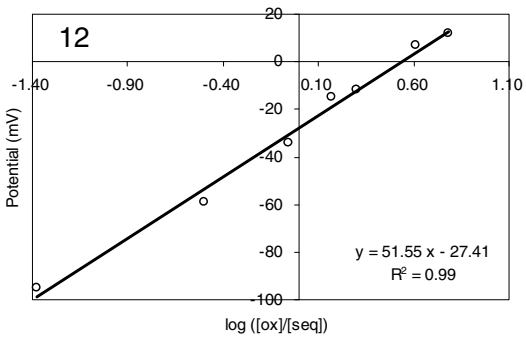

7
Potential (mV)
log ([seq]/[red])
y = 56.317x - 169.48
R² = 0.9652

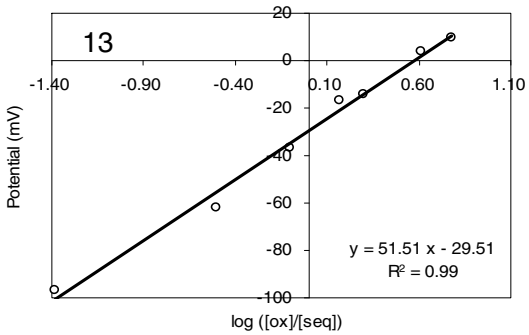

8
Potential (mV)
log(ox/red)
y = 27.09 x - 206.56
R² = 0.97

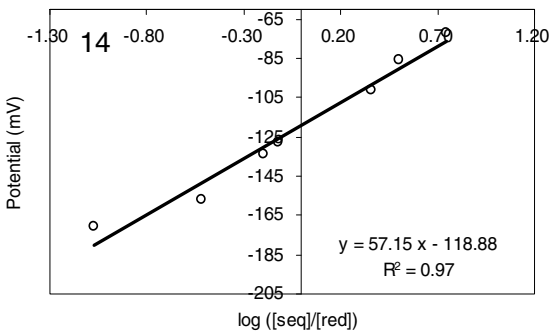

9
Potential (mV)
log(ox/red)
y = 27.47 x - 215.15
R² = 0.96

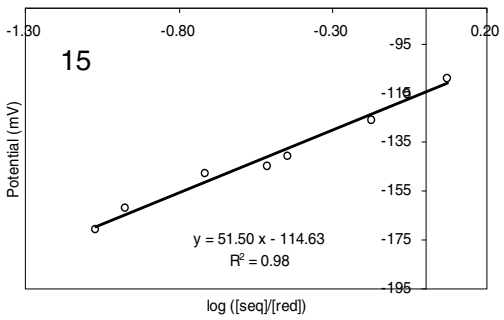

10
Potential (mV)
log(ox/red)
y = 29.93 x - 214.73
R² = 0.91

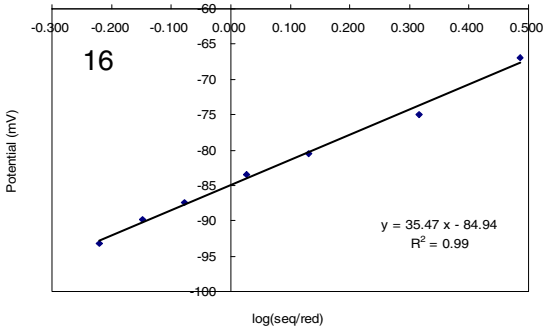

11
Potential (mV)
log(ox/red)
y = 27.61 x - 218.17
R² = 0.95

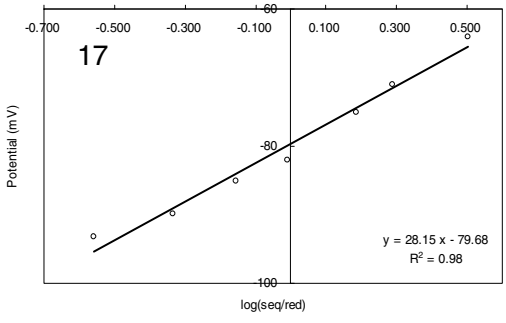

12
Potential (mV)
log ([ox]/[seq])
y = 51.55 x - 27.41
R² = 0.99

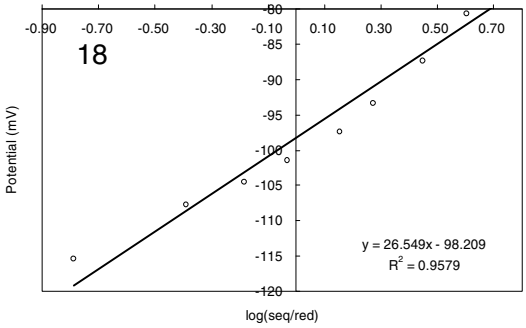

13
Potential (mV)
log ([ox]/[seq])
y = 51.51 x - 29.51
R² = 0.99


14
Potential (mV)
log ([seq]/[red])
y = 57.15 x - 118.88
R² = 0.97


15
Potential (mV)
log ([seq]/[red])
y = 51.50 x - 114.63
R² = 0.98


16
Potential (mV)
log(seq/red)
y = 35.47 x - 84.94
R² = 0.99


17
Potential (mV)
log(seq/red)
y = 28.15 x - 79.68
R² = 0.98


18
Potential (mV)
log(seq/red)
y = 26.549x - 98.209
R² = 0.9579

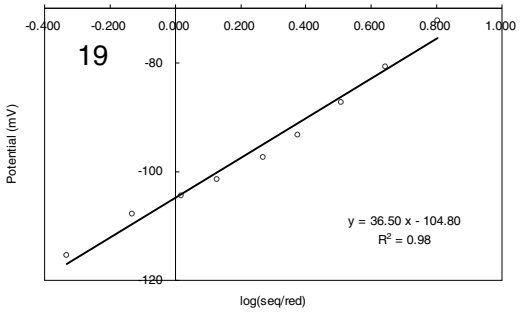

19
Potential (mV)
log(seq/red)
y = 36.50 x - 104.80
R² = 0.98

Figure S1. Nernst plots for redox potential titrations. The enzyme and corresponding redox indicator dye used are (at pH 7.0 unless otherwise stated): 1-2) WT and I2S; 3-4) WT and ANQ; 5) WT and CV; 6-7) WT and ANQ; 8-9) N485D and riboflavin; 10-11) N485L and riboflavin; 12-13) WT and I4S at pH 5.1; 14-15) WT and CV at pH 5.1; 16) N485D and riboflavin at pH 5.1; 17) N485D and CV at pH 5.1; 18) N485L and riboflavin at pH 5.1; 19) N485L and CV at pH 5.1.