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Citation
Journal of Biological Chemistry (JBC), 291(29): 15320-15331

Issue Date
2016-07-15

Doc URL
http://hdl.handle.net/2115/66637

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Energetic Mechanism of Cytochrome c-Cytochrome c Oxidase Electron Transfer Complex Formation under Turnover Condition Revealed by Mutational Effects and Docking Simulation

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*Running title: Energetic Analysis of Interactions between Cyt c and CcO

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Table of Contents:

Table S1 Interatomic distances (Å) between heme groups and its ligated amino acid residues     S-2

Table S2 Energetic contributions of Cyt c and each subunit of CcO                 S-3

Figure S1 Predicted binding interfaces of the Cyt c–CcO complexes of poses (a) 1, (b) 6, (c) 10, (d) 11, (e) 13, (f) 24, and (g) 25       S-4–S-5

Figure S2 CcO interaction site on wild type and Lys-13 → Leu mutant Cyt c.       S-6
**Table S1** Interatomic distances (Å) between heme groups and its ligated amino acid residues

![Diagram of protein structure with labeled distances](image)

<table>
<thead>
<tr>
<th>distance&lt;sup&gt;a&lt;/sup&gt;</th>
<th>protein (subunit)</th>
<th>observed&lt;sup&gt;b&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heme c@FE---His18@NE2</td>
<td>Cyt c</td>
<td>2.02 (0.06)</td>
</tr>
<tr>
<td>Heme c@FE---Met80@SD</td>
<td>Cyt c</td>
<td>2.30 (0.04)</td>
</tr>
<tr>
<td>Heme c@CAB---Cys14@SG</td>
<td>Cyt c</td>
<td>1.89 (0.09)</td>
</tr>
<tr>
<td>Heme c@CAC---Cys17@SG</td>
<td>Cyt c</td>
<td>2.13 (0.14)</td>
</tr>
<tr>
<td>Heme a@FE---His61@NE2</td>
<td>CcO (I)</td>
<td>1.95 (0.08)</td>
</tr>
<tr>
<td>Heme a@FE---His378@NE2</td>
<td>CcO (I)</td>
<td>1.95 (0.06)</td>
</tr>
<tr>
<td>Heme a3@FE---His376@NE2</td>
<td>CcO (I)</td>
<td>2.10 (0.11)</td>
</tr>
</tbody>
</table>

<sup>a</sup> See the insert figure.

<sup>b</sup> Average value and standard deviation (in parentheses). These values were obtained from the crystallographic structures of Cyt c and CcO (PDB codes: 1J3S, 3NWV, 3ZCF, and 3ZOO (Cyt c); 1OCR, 1OCT, 1V54, 1V55, 1OCC, 1OCC, 2Y69, 2ZXR, 2DYR, 2DYS, 2EIJ, 2EIK, 2EIL, 2EIM, 2EIN, 2OCC, 3ABM, 3AG1, 3AG2, 3AG3, 3AG4, 3ASN, 3ASO, 3ABK, and 3ABL (CcO)).
### Table S2 Energetic contributions of Cyt c and each subunit of CeO

<table>
<thead>
<tr>
<th>Protein (subunit)</th>
<th>$\Delta E_{vDW}^{a}$</th>
<th>$\Delta G_{\text{electro}}^{a,b}$</th>
<th>$\Delta G_{\text{nonpolar}}^{a}$</th>
<th>$\Delta G_{\text{tot}}^{a,c}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>wild-type Cyt c</td>
<td>−69.7</td>
<td>19.5</td>
<td>−12.5</td>
<td>−62.7</td>
</tr>
<tr>
<td>CeO (I)</td>
<td>−12.6</td>
<td>−5.6</td>
<td>−1.7</td>
<td>−20.0</td>
</tr>
<tr>
<td>CeO (II)</td>
<td>−9.7</td>
<td>−5.1</td>
<td>−1.7</td>
<td>−16.5</td>
</tr>
<tr>
<td>CeO (III)</td>
<td>−3.8</td>
<td>−1.2</td>
<td>−0.6</td>
<td>−5.6</td>
</tr>
<tr>
<td>CeO (IV–XIII)</td>
<td>−43.6</td>
<td>17.9</td>
<td>−6.7</td>
<td>−32.4</td>
</tr>
</tbody>
</table>

$^{a}$ In kcal/mol.

$^{b}$ $\Delta E_{\text{coul}} + \Delta G_{\text{polar}}$.

$^{c}$ $\Delta E_{vDW} + \Delta E_{\text{coul}} + \Delta G_{\text{polar}} + \Delta G_{\text{nonpolar}}$. 
Figure S1  Predicted binding interfaces of the Cyt $c$–CcO complexes of poses (a) 1, (b) 6, (c) 10, (d) 11, (e) 13, (f) 24, and (g) 25. The contact residues in subunits I, II, and III of CcO are represented in green, cyan, and magenta surfaces, respectively. Dashed lines indicate the heme $c$–Trp104 distances.
Figure S2. CcO interaction site on wild type and Lys-13 → Leu mutant Cyt c. Wild type (left) and Lys13 → Leu mutant Cyt c (right). The amino acid residues showing significant chemical shift perturbations associated with the binding CcO ($\Delta\delta > 0.020$ or line broadening) are highlighted.