

	Q <sub>o</sub>		Q <sub>i</sub>		
	SMA	HDQ	SMA	HDQ	Ubiquinone
<b>GOLDScore Range</b>	72.9-111.6	61.3-65.3	23.2-60.0	50.0-59.4	46.8-50.4
<b>Average</b>	<b>92.29</b>	<b>63.49</b>	<b>45.35</b>	<b>54.06</b>	<b>48.27</b>
<b>SD</b>	13.84	1.26	12.97	3.50	1.34
<b>ChemScore Range</b>	47.8-57.7	35.8-39.3	18.7-33.3	23.3-30.7	14.5-25.4
<b>Average</b>	53.97	37.71	28.03	28.63	22.24
<b>SD</b>	3.38	1.22	4.705	2.08	3.81
<b>Best solution</b>	GS=111.6 CS=57.2	GS=65.3 CS=35.8	GS=56.3 CS=33.3	GS=59.4 CS=29.8	GS=50.4 CS=25.0

**Table S1.** GoldScore results and associated data for the *in silico* docking of stigmatellin (SMA), HDQ and ubiquinone-6 at the Q<sub>o</sub>- and Q<sub>i</sub> sites of yeast *bc*<sub>1</sub> (3CX5.pdb). Dockings were performed with GOLD 5.0.1 as described in Materials and Methods.