

# Terminal Electron-Proton Transfer Dynamics in the Quinone Reduction of Respiratory Complex I

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**Figure S11.** Models employed for the QM/MM MD simulations. A) QM/MM model with subunits Nqo4, Nqo5, Nqo6, Nqo7, Nqo8 and Nqo9 of complex I (PDB ID:4HEA). The models comprise the quinone, and ISCs N2, N6A, and N6B B) QM part of the QM/MM models. The N2 subsystem (within dotted black lines), the QM model of the Q subsystem (within dotted blue lines), and the combined N2/Q system (within dotted red lines).

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Figure S14. Comparison of the calculated pH dependent redox potential for N2 for the wild type structure, and for the H169M and R84A mutations in subunit Nqo4. The calculated and measured values at pH=7 were set equal. Experimental data obtained from.<sup>1</sup>

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Figure S17. Water molecules surrounding Q and the ISCs after 100 ns classical MD simulations of complex I. The blue surface represents the Q while N2 and N6B are shown as yellow surfaces. Several histidine and serine residues surround the cofactors, and could help in providing water wires to the bulk solvent from the hydrophilic domain of complex I. Data from.<sup>2</sup>

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Table S4. Comparison of redox potentials calculated for a large (E<sub>m</sub><sup>1</sup>) and small (E<sub>m</sub><sup>2</sup>) complex I setups. Coordinates were obtained from a 1 ns relaxation of all subunits of complex I crystal structure while UQ was modelled in the hydrogen-bonded conformation. C $\beta$  atoms were fixed. FMN, N1B, N4, N5, N6A, N6B, N2 and quinone (UQ) were modelled as titratable redox groups. N1A and N3 were fixed in the reduced state, while N7 and FMN were fixed in the oxidized state. Lys, Arg, His, Glu, Asp, Tyr and Cys were considered as titratable residues, and all other protein atoms were treated explicitly with atomic partial charges in a low dielectric constant, while water was treated as a continuum with high dielectric constant. We considered nine (five) conformations for the large (small) system prepared with different alternated oxidation states of the cofactors by optimizing only hydrogen-atom positions. Redox potentials are reported as Poisson-Boltzmann average of these conformations. The intrinsic error of these calculations ranges from ca. 60 mV for organic compounds<sup>7</sup> to ca. 200 mV for ISC.<sup>8</sup>

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Tables S6. Coordinates of the N2 cluster and ubiquinone (UQ)/menaquinone (MQ), in different oxidation states, optimized at the B3LYP-D3 level, employing the def2-TZVP (S, Fe) and def2-SVP (H, C, N, O) basis sets, using the COSMO solvation model with  $\epsilon=4$ , along with SCF energies using the def2-TZVPP basis set. Standard XYZ format in Ångström units, energies [E] in Hartree. Atoms marked with an asterisk (\*) were kept frozen during the geometry optimization procedure.

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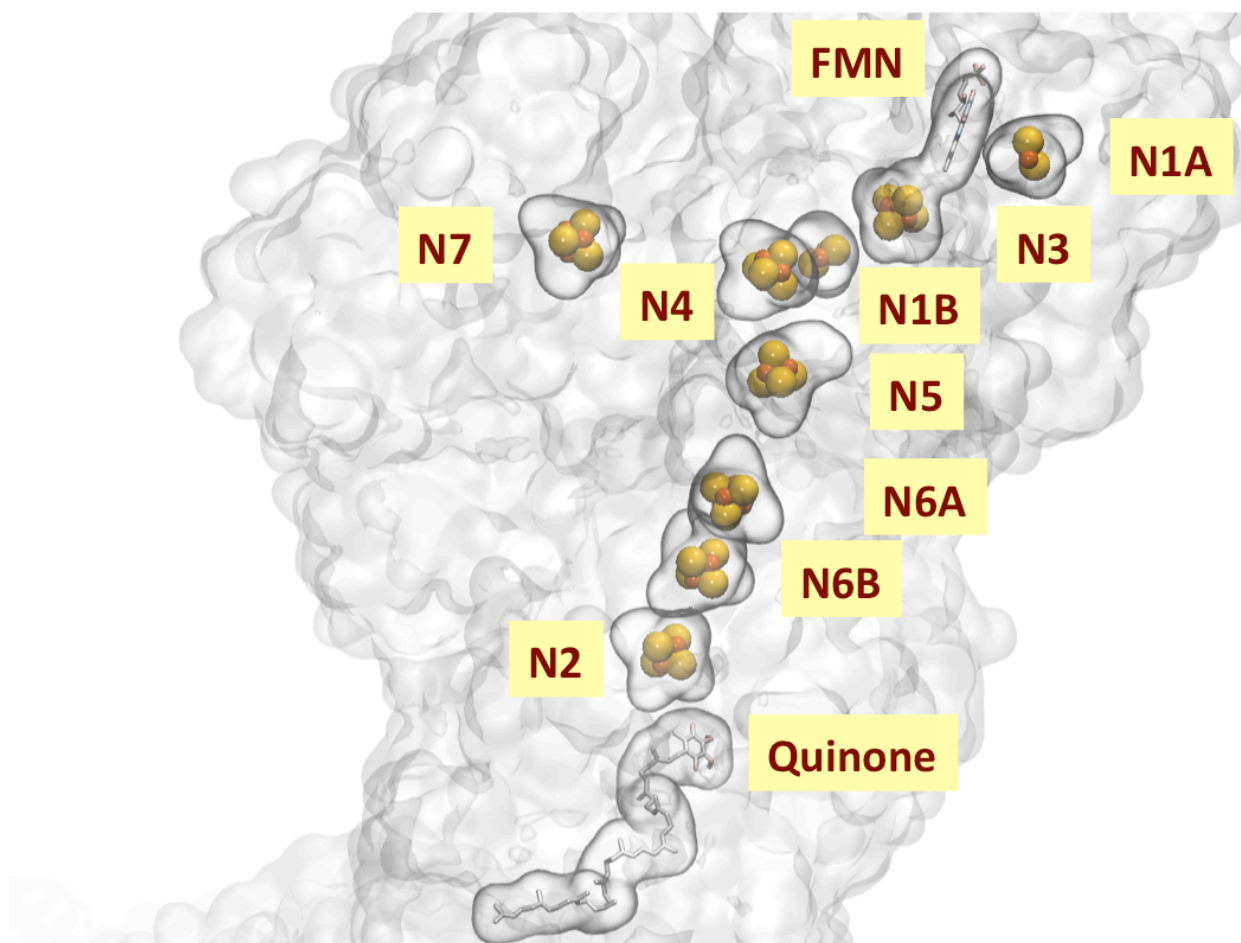
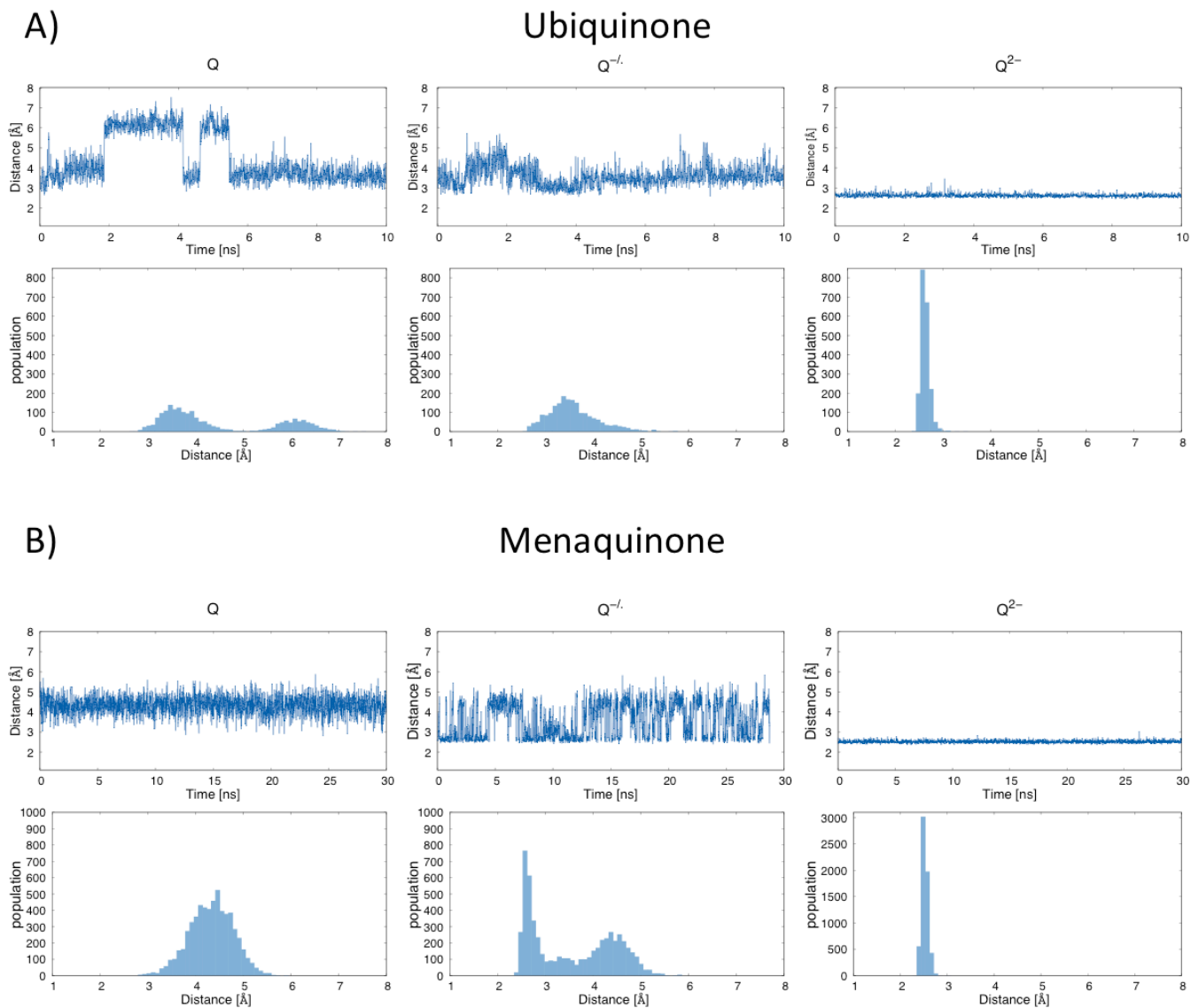


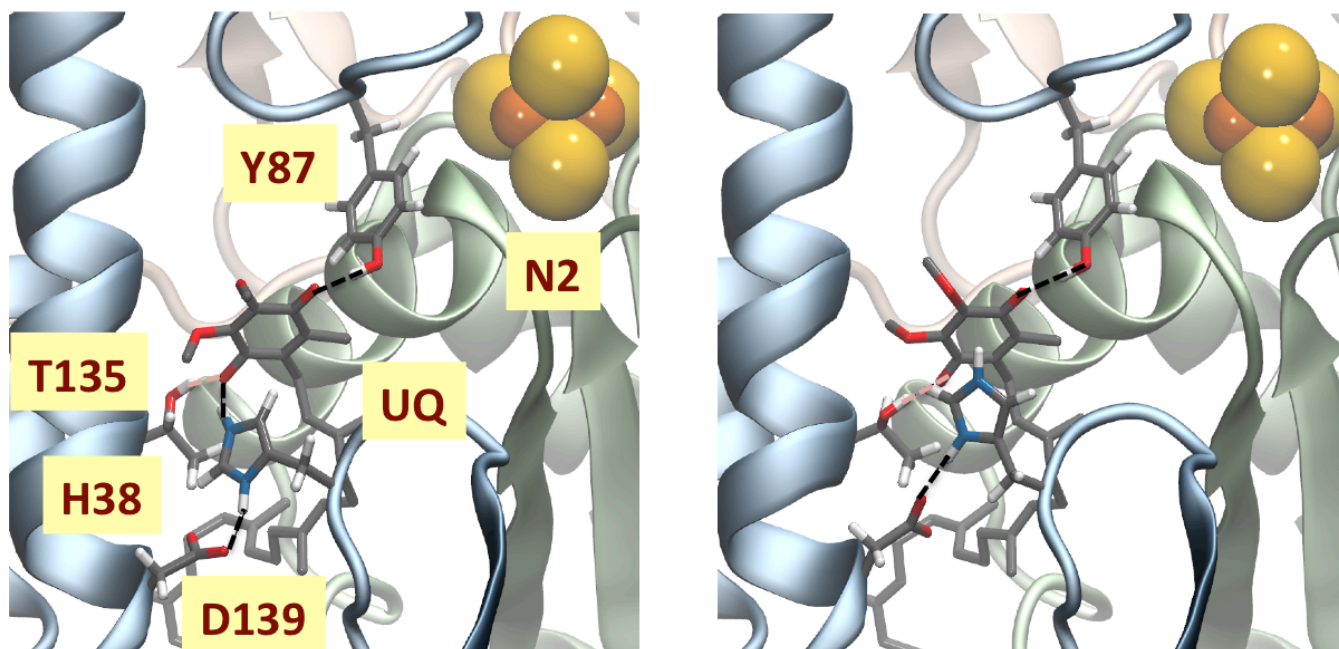
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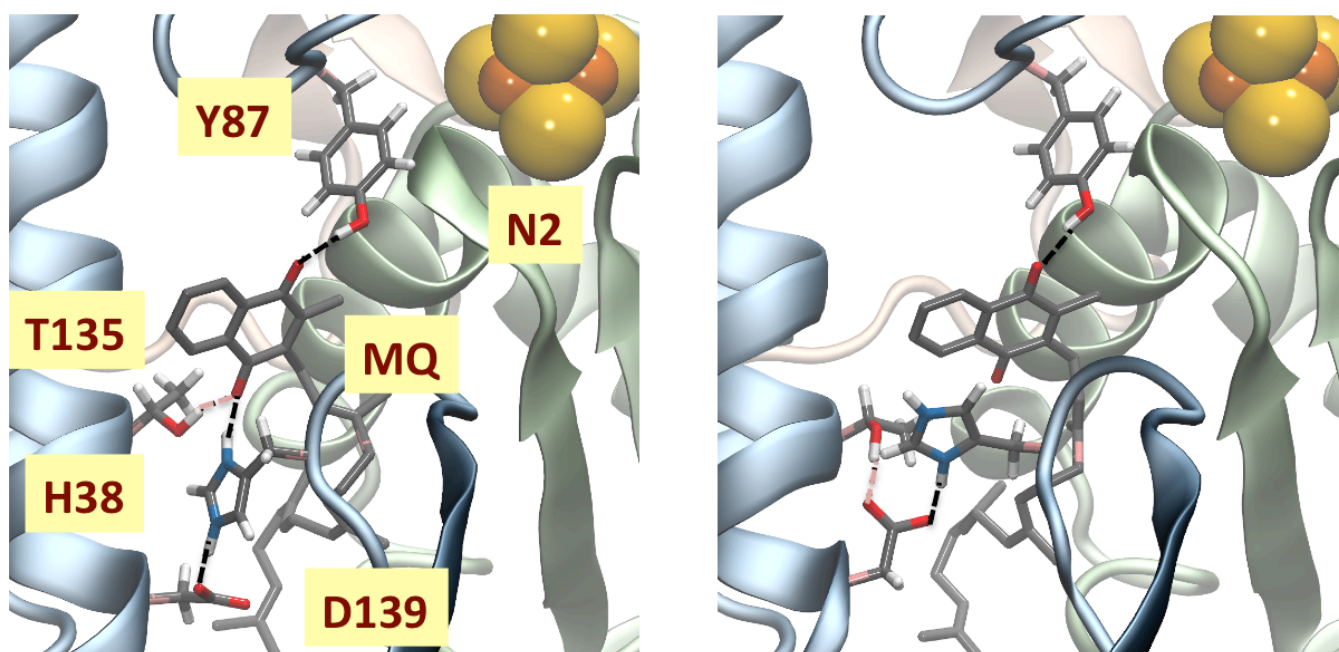
A)

## Ubiquinone



B)

## Menaquinone



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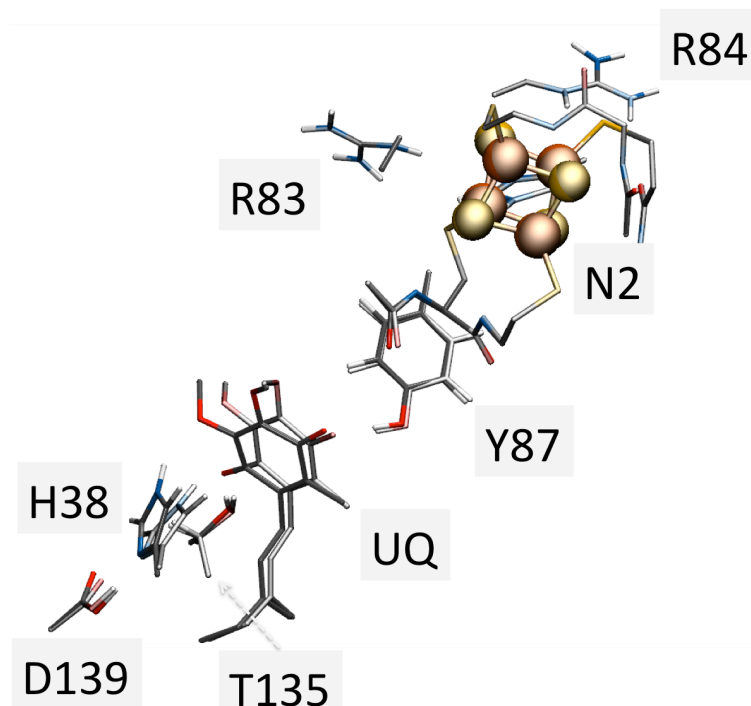


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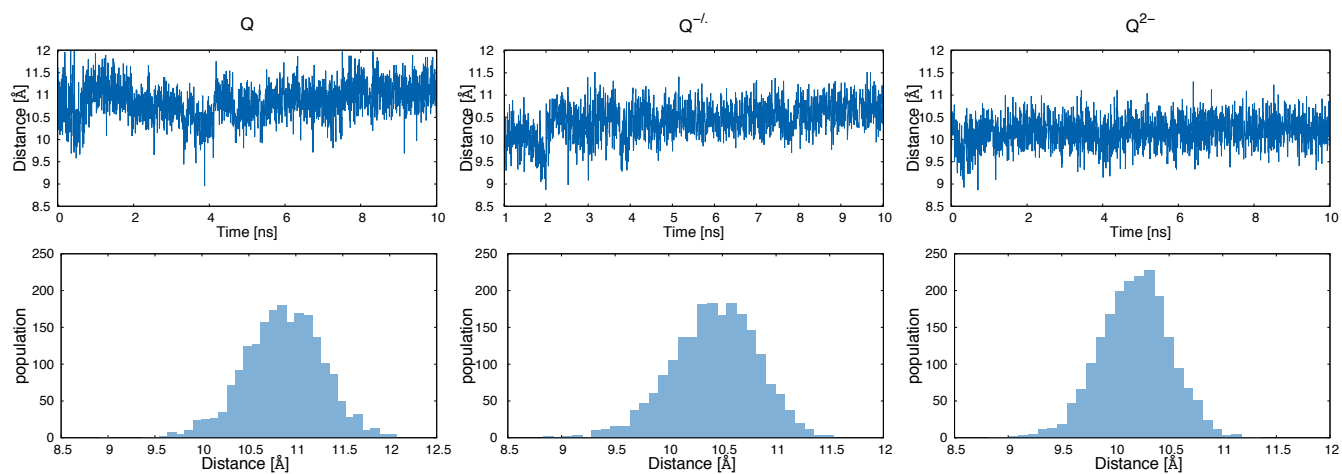
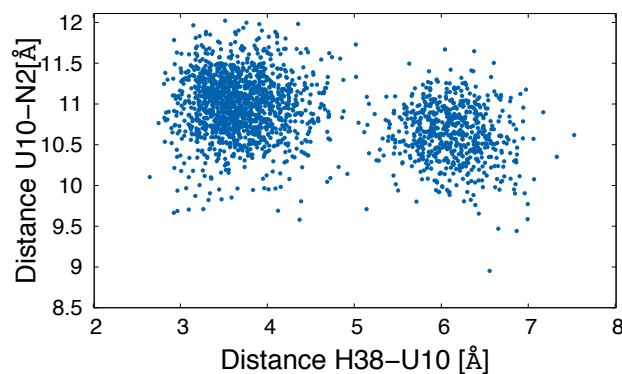
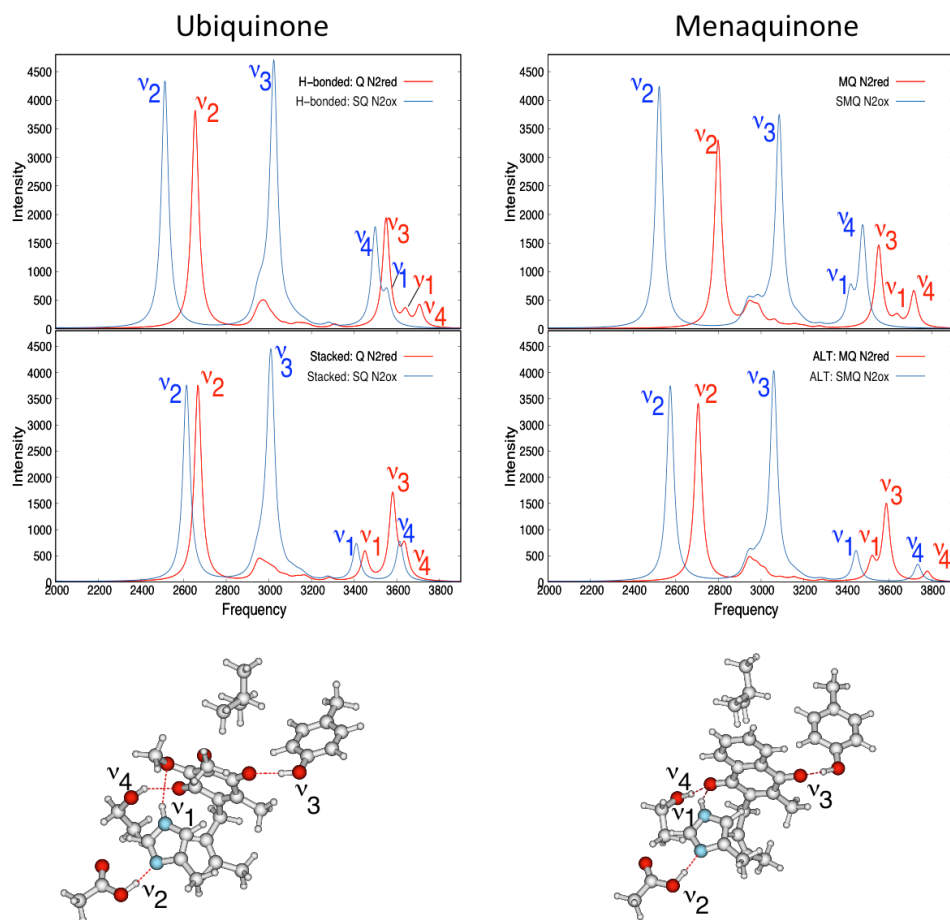


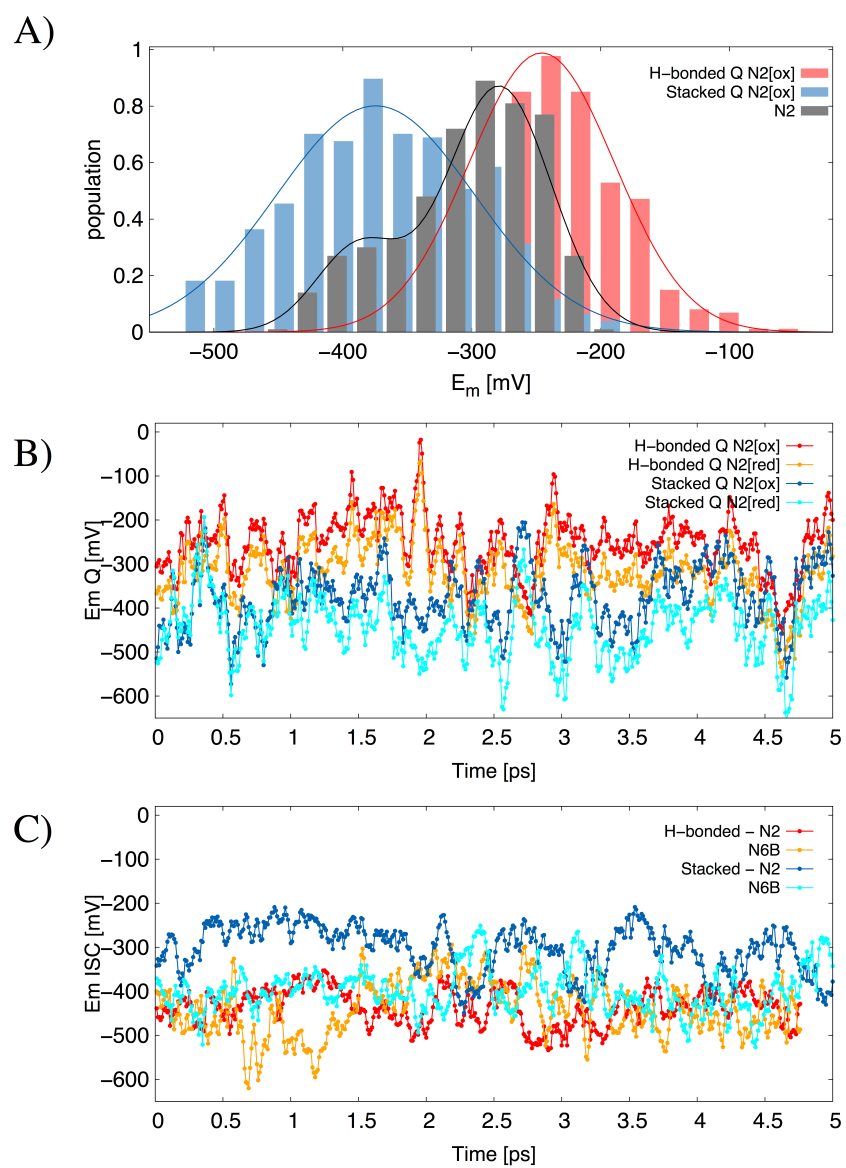
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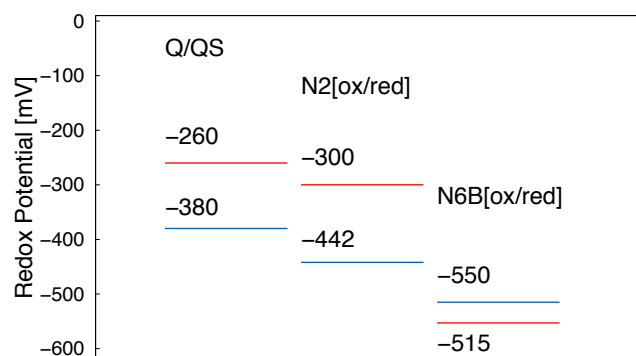


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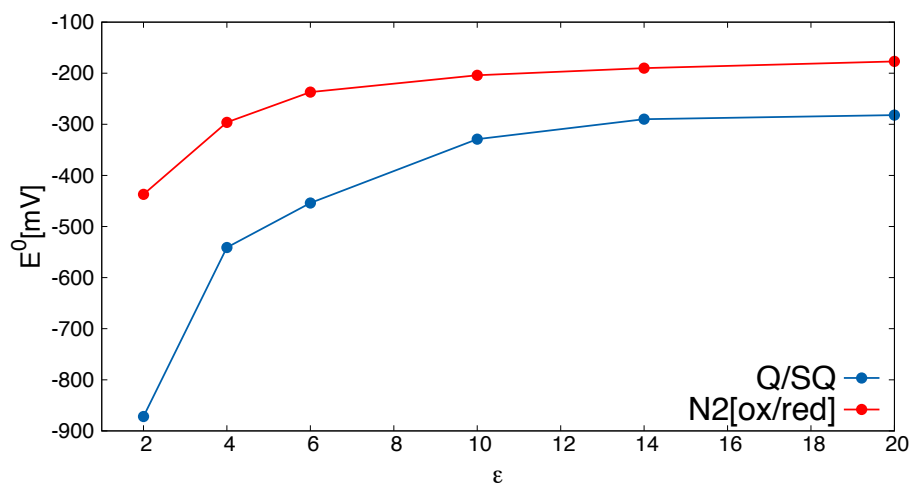
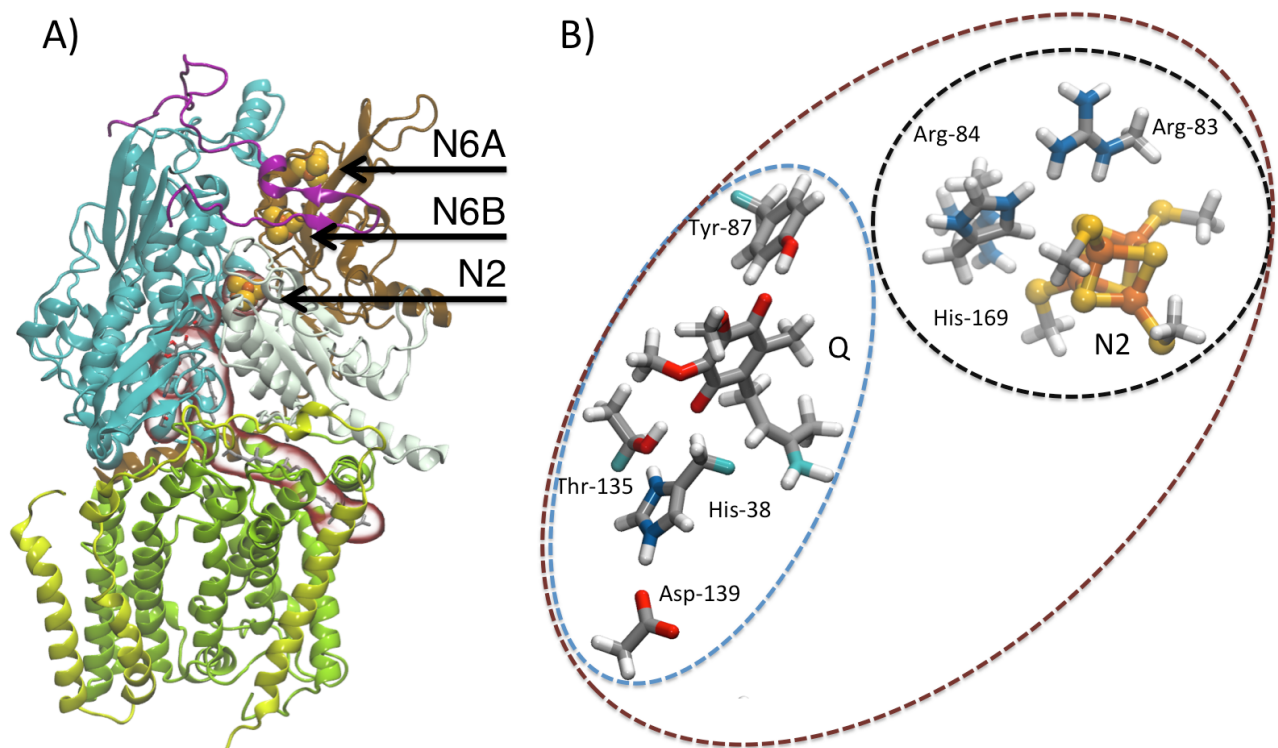


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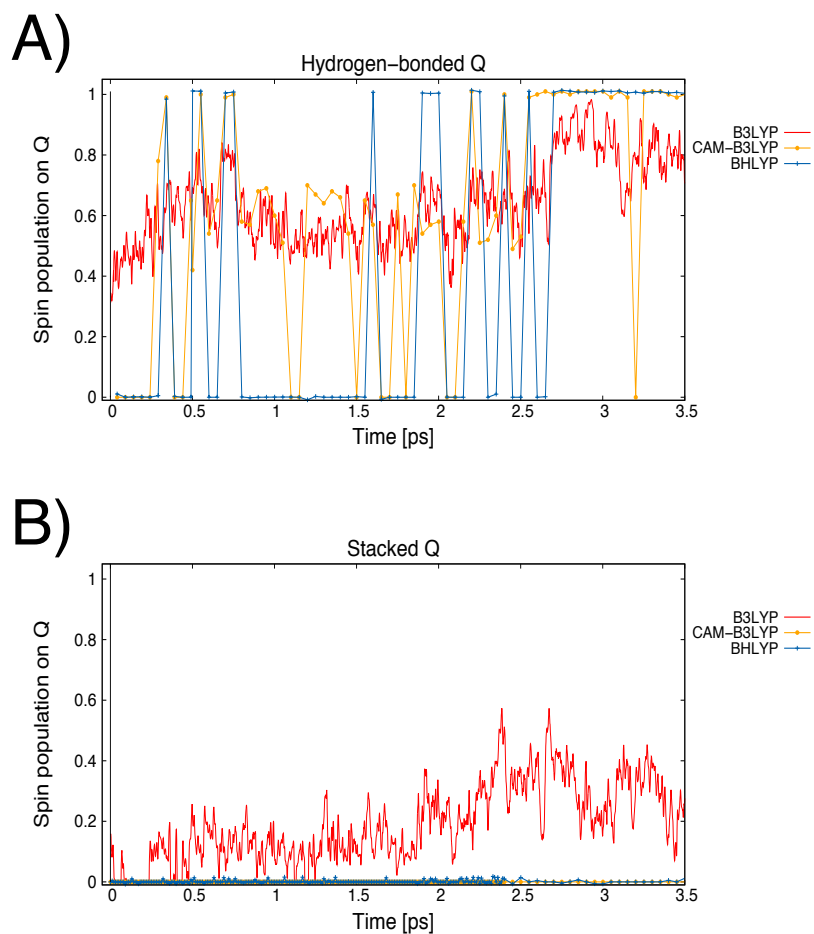


Figure S12. QM/MM dynamics of the electron transfer between N2 and Q in A) the hydrogen-bonded and B) the stacked conformations. Comparison of the total Mulliken spin population on Q obtained at DFT level, by employing different density functionals (B3LYP, CAM-B3LYP, BHLYP).

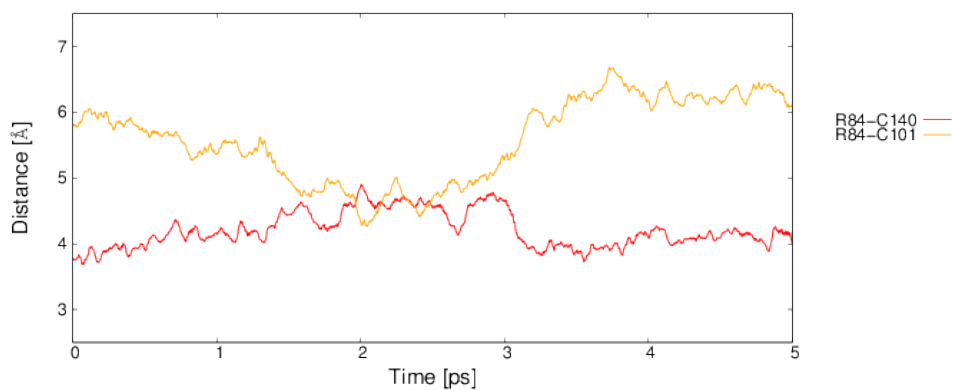


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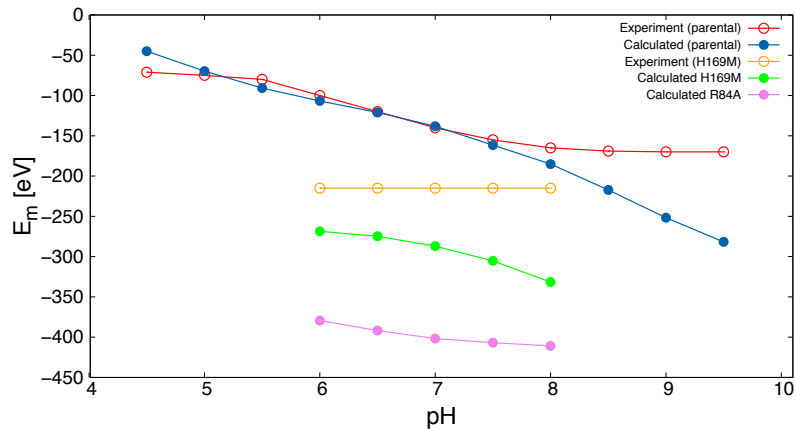


Figure S14. Comparison of the calculated pH dependent redox potential for N2 for the wild type structure, and for the H169M and R84A mutations in subunit Nqo4. The calculated and measured values at pH=7 were set equal. Experimental data obtained from.<sup>1</sup>

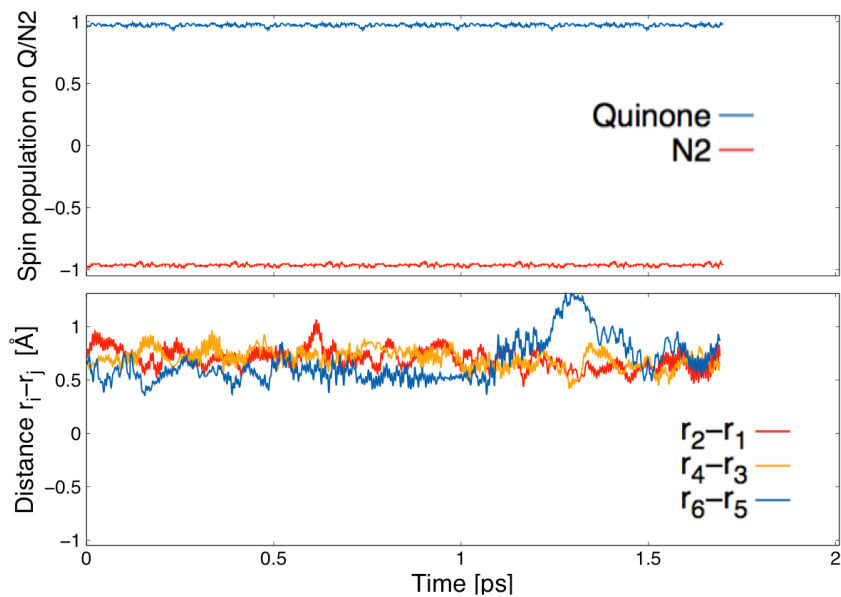


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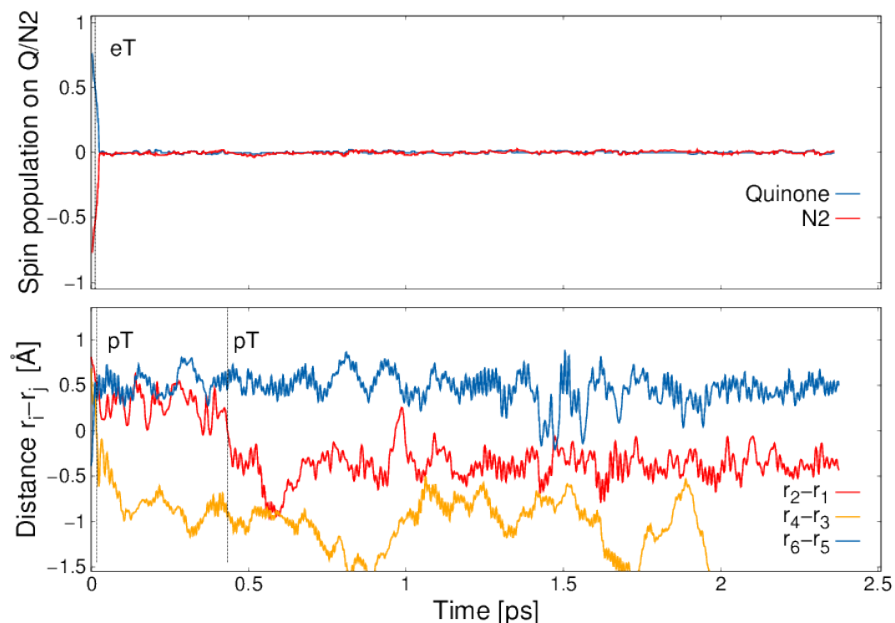


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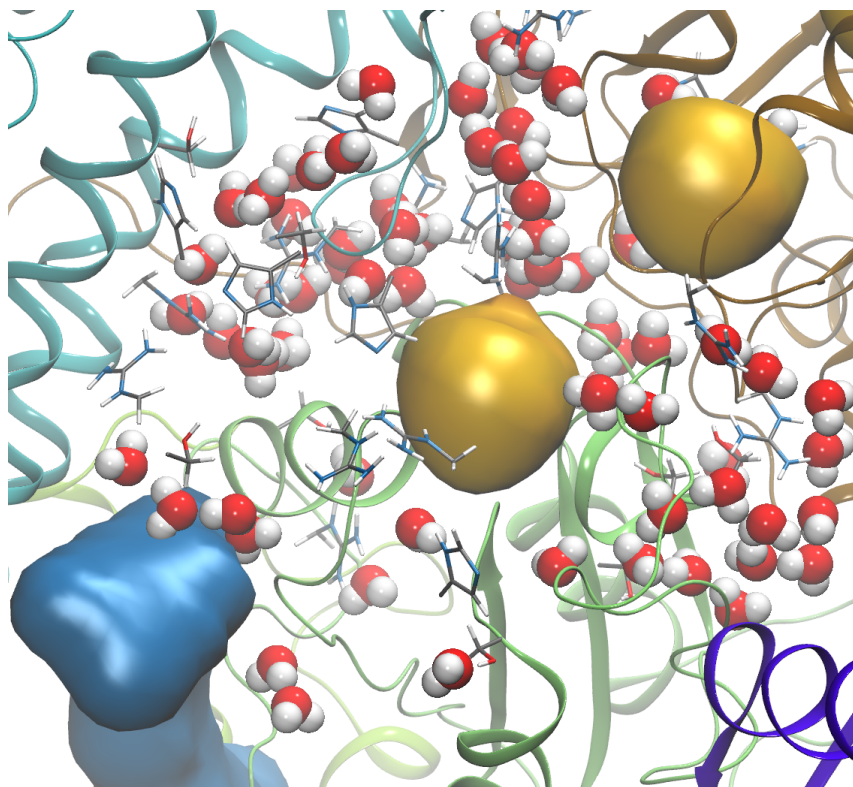
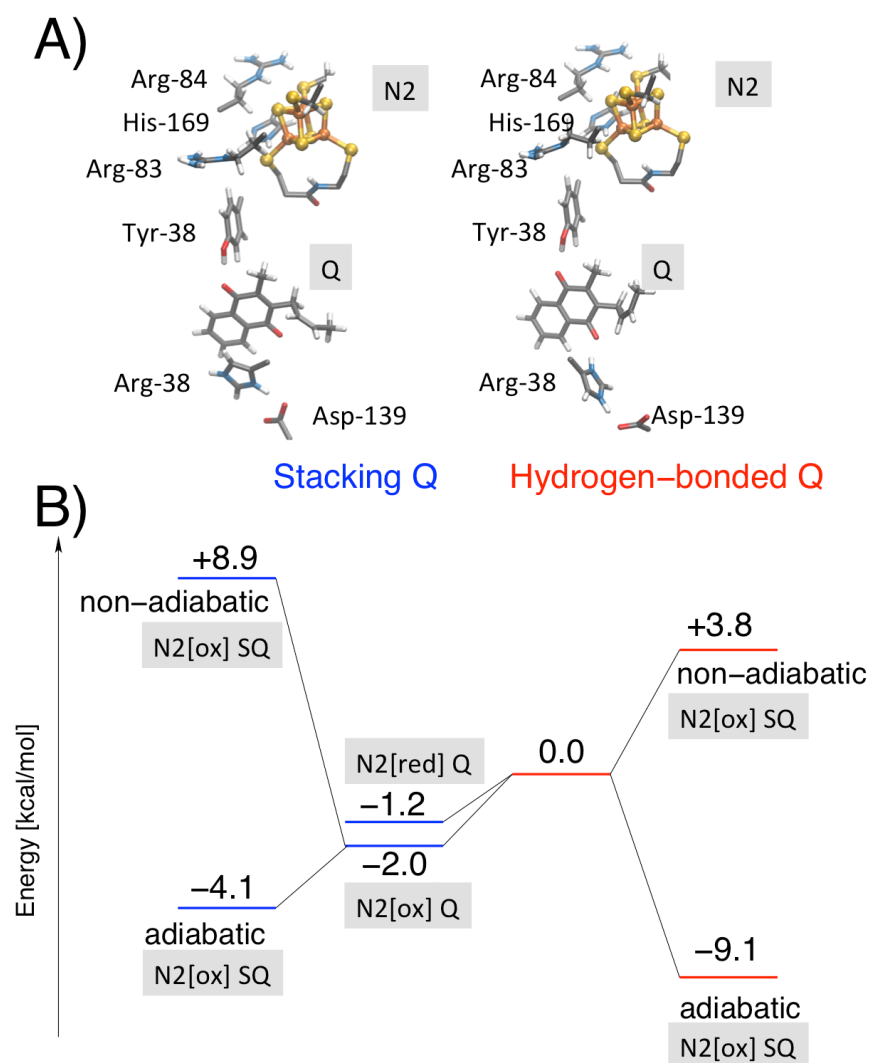


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**Figure S18.** *A) Structure and B) B3LYP-D3/def2-TZVPP/ $\epsilon=4$  energetics (in kcal mol<sup>-1</sup>) of hydrogen-bonded (right) and stacked (left) binding modes of menaquinone (MQ) in complex I. Q and SQ refer to oxidized and semiquinone species, while N2[ox] and N2[red] refer to oxidized (2Fe[II]2Fe[III]) and reduced (3Fe[II]1Fe[III]) states of N2, respectively. Non-adiabatic and adiabatic electron transfer energetics are calculated by relaxing the initial electron donor state (N2/Q), or by relaxing both the initial (N2[red]/Q) and final (N2[ox]/SQ) states, respectively.*

**Table S1. Energetics of Q-binding and electron transfer between N2 and UQ at the DFT B3LYP-D3/def2-TZVPP/ $\epsilon=4$  and TPSSH-D3/def2-TZVPP/ $\epsilon=4$  levels (in parenthesis). Q and SQ refer to oxidized and semiquinone states, respectively; N2[ox] and N2[red] refer to oxidized (2Fe[II]2Fe[III]) and reduced (3Fe[II]1Fe[III]) states of N2, respectively. Non-adiabatic and adiabatic electron transfer energetics are calculated by relaxing the initial electron donor state (N2/Q), or by relaxing both the initial (N2[red]/Q) and final (N2[ox]/SQ) states, respectively.**

State/System		H-bonded (kcal·mol <sup>-1</sup> )	Stacked (kcal·mol <sup>-1</sup> )	
Q/N2[ox]		0.0 (0.0)	-2.0 (-2.0)	
Q/N2[red]		0.0 (0.0)	-3.0 (-2.9)	
SQ/N2[ox]		0.0 (0.0)	+1.9 (2.2)	
Q/N2[red]	non-adiabatic	+5.2 (2.5)	+11.2 (8.6)	
SQ/N2[ox]	adiabatic	-8.5 (-13.6)	-3.6 (-8.4)	
		$E_m$ (mV)	$E_m$ (mV)	<i>Exp.</i> $E_m$ (mV) <sup>c</sup>
N2[ox]/N2[red]			-34 <sup>a</sup>	-50... -150 <sup>3,4</sup>
N4[ox]/N4[red]			-250 <sup>a</sup>	-250 <sup>3,4</sup>
Q/SQ		0 <sup>b</sup>	-168 <sup>b</sup>	< -300 <sup>5</sup>

<sup>a</sup> Electron affinity of N4 set to the experimental value, and the electron affinity N2 value calculated based on the shifts.

<sup>b</sup> Relative shift of the stacked conformation with respect to the hydrogen-bonded conformation.

<sup>c</sup> Experimental redox potentials of UQ and N2 are reported from *E. coli* and due to sequence similarity, their relative shifts can be expected to be similar to *T. thermophilus*, whose  $E_m$  values have not been determined.<sup>6</sup>

**Table S2. Energetics of MQ-binding and electron transfer between N2 and MQ at the DFT B3LYP-D3/def2-TZVPP/ $\epsilon=4$ . Q and SQ refer to oxidized and semiquinone states, respectively; N2[ox] and N2[red] refer to oxidized (2Fe[II]2Fe[III]) and reduced (3Fe[II]1Fe[III]) states of N2, respectively. Non-adiabatic and adiabatic electron transfer energetics are calculated by relaxing the initial electron donor state (N2/Q), or by relaxing both the initial (N2[red]/Q) and final (N2[ox]/SQ) states, respectively.**

State/System		H-bonded (kcal mol <sup>-1</sup> )	Stacked (kcalmol <sup>-1</sup> )
MQ/N2[ox]		0.0	-1.4
MQ/N2[red]		0.0	-1.2
SQ/N2[ox]		0.0	+5.8
Q/N2[red]	non-adiabatic	+3.8	+10.1
SQ/N2[ox]	adiabatic	-9.1	-2.1

**Table S3. Redox state-dependence of the pK<sub>a</sub> of His-169. The table shows the pK<sub>a</sub> values of His-169 obtained by PB electrostatics of the hydrogen-bonded and stacked conformations of Q, while maintaining the redox state of the N2 cluster fixed to the oxidized (N2[ox]) or reduced (N2[red]) state, respectively.**

State/System	H-bonded (pK <sub>a</sub> units)	Stacked (pK <sub>a</sub> units)
Q/SQ w. N2[ox]	13.0	6.8
Q/SQ w. N2[red]	48.0	22.3

**Table S4. Comparison of redox potentials calculated for a large ( $E_m^1$ ) and small ( $E_m^2$ ) complex I setups. Coordinates were obtained from a 1 ns relaxation of all subunits of complex I crystal structure while UQ was modelled in the hydrogen-bonded conformation. Ca atoms were fixed. FMN, N1B, N4, N5, N6A, N6B, N2 and quinone (UQ) were modelled as titratable redox groups. N1A and N3 were fixed in the reduced state, while N7 and FMN were fixed in the oxidized state. Lys, Arg, His, Glu, Asp, Tyr and Cys were considered as titratable residues, and all other protein atoms were treated explicitly with atomic partial charges in a low dielectric constant, while water was treated as a continuum with high dielectric constant. We considered nine (five) conformations for the large (small) system prepared with different alternated oxidation states of the cofactors by optimizing only hydrogen-atom positions. Redox potentials are reported as Poisson-Boltzmann average of these conformations. The intrinsic error of these calculations ranges from ca. 60 mV for organic compounds<sup>7</sup> to ca. 200 mV for ISC.<sup>8</sup>**

		Ubiquinone		
		Large setup $E_m^1$ [mV]	Small setup $E_m^2$ [mV]	$\Delta E_m^{2-1}$ [mV]
UQ/SQ	-290	-337	+47	
N2	-546	-563	+17	
N6B	-447	-445	-2	
N6A	-555	-452	-103	
N5	-187			
N4	-625			
N1B	-626			
N3	-466			



**Table S5. Calculated redox potentials for quinone (Q/SQ) model compounds [ $E_m$  mV vs. SHE] used in PBE calculations in the protein.  $E_m$  values for UQ and MQ were calculated within the protein environment. Conversion from SCE electrode to SHE values were obtained by adding + 241 mV to the SCE potentials.<sup>10</sup>**

	Experiment <sup>9</sup>		Calculated <sup>a</sup>		
	DMF SCE	DMF SHE	DMF SHE	water cal+shift	Protein
Benzoquinone	-401	-157	-150	30	-
Plastoquinone	-640	-396	-365	-178	-
Ubiquinone	-611	-367	-367	-188	-260/-380 <sup>b</sup>
Menaquinone	-709	-465	-414	-241	-230/-690 <sup>b</sup>
	RMSD		57 mV		

<sup>a</sup> B3LYP/def2-TZVP (DMF  $\epsilon=36.7$ , 2.54 Å probe radius and water  $\epsilon=80$ , 1.4 Å probe radius).

Values set to match experiment/calculated ubiquinone  $E_m$ .

<sup>b</sup> Calculated redox potentials for complex I with quinone (UQ/MQ) considering subunits Nqo4, Nqo5, Nqo6, Nqo7, Nqo8 and Nqo9. Coordinates were obtained from a 1 ns relaxation with all subunits of complex I from the crystal structure with UQ/MQ modeled in both, hydrogen-bonded and stacked conformations while fixing C $\beta$  atoms. N6A, N6B, N2 and UQ/MQ were modeled as titratable redox groups and Lys, Arg, His, Glu, Asp, Tyr and Cys were considered as titratable residues, and all other protein atoms were treated explicitly with atomic partial charges in a low dielectric constant, while water was treated as a continuum with high dielectric constant. We considered nine conformations for a system prepared with different alternated oxidation states of the cofactors by optimizing only hydrogen-atom positions. Redox potentials are reported as Poisson-Boltzmann average of these conformations.

**Tables S6. Coordinates of the N2 cluster and ubiquinone (UQ)/menaquinone (MQ), in different oxidation states, optimized at the B3LYP-D3 level, employing the def2-TZVP (S, Fe) and def2-SVP (H, C, N, O) basis sets, using the COSMO solvation model with  $\epsilon=4$ , along with SCF energies using the def2-TZVPP basis set. Standard XYZ format in Ångström units, energies [E] in Hartree. Atoms marked with an asterisk (\*) were kept frozen during the geometry optimization procedure.**

**Table S6.1 Ubiquinone stacked, Q N2[red]**

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211
# E=-12375.75482706 Hartree
C 70.47811 -25.30041 32.97933
C 71.51341 -24.48514 32.26029
C 72.80006 -24.17905 32.92676
C 72.96296 -24.42744 34.25865
C 71.88964 -25.19043 34.99028
C 70.64562 -25.60795 34.29040
C 69.29049 -25.65781 32.14337
C 74.30876 -24.11593 31.05749
C 75.08611 -23.30652 34.62175
C 69.64704 -26.38842 35.12094
C 69.92813 -27.87449 35.08511
C 69.11973 -28.84101 34.62532
C 67.73926 -28.70494 34.04961
O 71.29694 -24.07345 31.12864
O 73.72778 -23.48196 32.20902
O 73.98048 -24.11357 35.05350
O 72.07109 -25.45108 36.17374
C* 67.23998 -22.83799 33.62699
C 69.71422 -22.24746 34.16432
C 68.51039 -22.05982 33.51281
N 70.56897 -21.27840 33.68082
N 68.64108 -20.98968 32.65039
C 69.88320 -20.55191 32.77323
C* 76.92097 -28.86699 39.93099
C 75.57329 -28.54271 39.34205
C 75.40518 -27.45860 38.46847
C 74.15470 -27.12586 37.94179
C 73.02566 -27.88974 38.28499
O 71.78085 -27.60774 37.83320
C 74.43747 -29.30834 39.65684
C 73.18124 -28.99460 39.14027
C* 77.29698 -23.20700 40.02999
C* 76.39197 -23.68199 38.88999
C* 75.38298 -22.57599 38.53599
C* 77.16697 -24.08299 37.64199
C 73.12438 -20.02228 31.84349
O 73.28319 -20.89944 32.96191
C* 72.55898 -20.73499 30.62099
C* 67.48798 -17.76800 29.31099
C 68.16611 -18.68038 30.30415
O 67.32773 -19.53616 30.86211
O 69.35905 -18.61354 30.55690
H 68.53380 -26.22653 32.69278
H 69.61243 -26.25310 31.27306
H 68.83689 -24.74083 31.73505
H 75.07886 -23.42585 30.68861
H 73.55156 -24.28226 30.27955
H 74.77776 -25.07014 31.34825
H 75.71512 -23.18426 35.50821
H 74.74482 -22.32159 34.27714
H 75.65623 -23.80826 33.82735
H 69.71513 -26.03512 36.16243
H 68.62827 -26.16634 34.77933
H 70.90306 -28.16502 35.48966
H 69.50220 -29.86876 34.67461
H 67.33549 -27.68368 34.11639
H 67.03470 -29.37651 34.57015
H 67.72697 -29.00588 32.98674
H 66.40711 -22.20198 33.97095
H 67.35162 -23.67025 34.33837
H 66.94703 -23.25720 32.65006
H 70.01190 -22.96510 34.92195
H 71.58681 -21.19443 33.79979
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H 77.63512 -28.04490 39.76964

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H	77.37544	-29.76954	39.49500
H	76.84092	-29.01120	41.02240
H	76.27094	-26.84966	38.19327
H	74.04599	-26.27025	37.27115
H	71.79507	-26.79771	37.28427
H	74.53363	-30.16992	40.32569
H	72.30005	-29.58878	39.39383
H	78.02001	-23.98605	40.32625
H	76.70657	-22.93647	40.92104
H	77.87471	-22.31534	39.72715
H	75.82724	-24.56495	39.24269
H	75.90723	-21.67729	38.16587
H	74.78388	-22.27744	39.41231
H	74.68244	-22.90605	37.75020
H	77.66200	-23.21026	37.18093
H	76.50147	-24.53641	36.89136
H	77.95241	-24.82444	37.86899
H	72.45294	-19.21147	32.17052
H	74.09247	-19.54654	31.59335
H	73.57641	-21.76364	32.61130
H	71.66293	-21.31894	30.87573
H	73.29744	-21.43270	30.19347
H	72.28556	-20.00414	29.84367
H	68.22318	-17.10009	28.84504
H	66.71525	-17.17570	29.82684
H	66.97610	-18.36664	28.54112
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.03184	-36.07945	44.79388
N	80.33217	-36.53247	44.31381
C	81.48238	-36.42027	44.98183
N	81.48935	-36.19745	46.30890
N	82.63283	-36.51890	44.30986
C*	75.72200	-32.17300	44.73700
O	74.77397	-32.92133	44.65263
C*	81.64500	-32.53700	42.95900
N	79.53125	-31.21432	42.41487
C	80.31381	-32.35701	42.33010
C	78.32512	-31.44864	41.87794
N	78.31595	-32.71011	41.45230
C	79.53510	-33.28581	41.69598
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39499	-33.61042	39.52035
C*	77.25800	-32.00400	36.55700
O	77.90270	-31.13843	35.95526
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.19925	-36.53253	35.38604
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.83522	-36.62366	41.36673
N	72.87115	-35.16431	41.23318
C	73.04336	-34.33565	42.26184
N	72.86817	-34.76948	43.51655
N	73.35994	-33.04822	42.03214
C*	79.04600	-41.17200	35.58000
O	78.32214	-41.96033	34.98257
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17259	-43.77572	37.76703
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.63144	-39.62866	40.69227
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62641	-39.31751	37.25122
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.47050	-36.21041	41.26910

Fe	76.98106	-37.96191	39.90386
Fe	78.44995	-36.93652	37.51450
Fe	76.90676	-35.38740	39.45690
Fe	79.33069	-36.51577	40.37500
S	79.00923	-34.85946	38.74600
S	77.29686	-36.32847	41.59982
S	79.06759	-38.58075	39.22281
S	76.11352	-36.95421	37.94201
H	77.53548	-32.13726	45.86551
H	77.75646	-32.11961	44.13511
H	77.02388	-34.55789	45.89084
H	76.76737	-34.59486	44.14083
H	79.54161	-34.05095	45.40362
H	79.16028	-34.25676	43.68287
H	78.85571	-36.43653	45.82264
H	78.28228	-36.57062	44.15722
H	80.43202	-36.66402	43.29292
H	82.36523	-36.18367	46.81734
H	80.64778	-36.34111	46.85334
H	82.58706	-36.48817	43.28105
H	75.57473	-31.06610	44.66231
H	73.54656	-32.46995	42.84478
H	82.06479	-33.50141	42.63866
H	81.55782	-32.54074	44.05866
H	82.34928	-31.73892	42.67565
H	79.81897	-30.32380	42.81261
H	77.51838	-30.72943	41.79303
H	77.52026	-33.20803	41.02752
H	79.75690	-34.30286	41.40387
H	75.25764	-31.74182	37.31252
H	76.44223	-30.50481	37.76421
H	76.57923	-31.57425	39.75743
H	77.57895	-32.76589	38.92719
H	76.86587	-34.00336	36.75961
H	77.69098	-33.27628	34.13300
H	79.14750	-33.57443	35.09131
H	77.94156	-35.49372	33.64150
H	76.92419	-35.70516	35.07175
H	71.73868	-37.81068	38.22577
H	71.26932	-36.24606	38.92739
H	70.75546	-37.75983	39.71333
H	73.72616	-36.88640	39.43436
H	73.16787	-38.34280	40.19816
H	73.71668	-36.94544	41.94871
H	71.92432	-36.92288	41.91708
H	72.99890	-34.77572	40.30185
H	72.60218	-35.72838	43.70034
H	73.27556	-34.23444	44.27744
H	73.92319	-32.87333	41.18713
H	79.40116	-40.21572	35.12707
H	80.14914	-40.63869	37.18277
H	79.45405	-43.43560	37.01810
H	79.84292	-41.43586	39.35711
H	81.14768	-42.33883	38.53528
H	79.95125	-43.21137	39.52893
H	77.53567	-40.73803	38.51807
H	75.31845	-42.32053	39.42824
H	75.07273	-41.92421	37.71420
H	74.02289	-40.15867	38.97690
H	75.46599	-39.46385	38.24703
H	83.52744	-36.52586	44.78335
H	83.25322	-41.34247	36.96953
H	84.05157	-40.07029	36.03429
H	84.67196	-40.48734	37.65728
H	84.35680	-38.59633	38.62894
H	81.84794	-37.06681	38.31985
H	83.13267	-37.92297	40.98073
H	81.55036	-38.44281	40.35819
H	83.41672	-36.44812	38.92381

Table S6.2 Ubiquinone stacked, Q N2[ox]

211

# E=-12375.61898974 Hartree

C	70.49998	-25.31811	32.92207
C	71.54162	-24.49956	32.21549
C	72.81978	-24.19033	32.89733
C	72.97177	-24.45020	34.22836
C	71.90176	-25.23562	34.93972
C	70.65707	-25.63347	34.23248
C	69.31159	-25.66076	32.08161
C	74.35014	-24.10359	31.04618
C	75.07703	-23.30717	34.62469
C	69.64351	-26.40837	35.05065
C	69.87679	-27.90071	34.97164
C	69.02011	-28.83155	34.52558
C	67.62228	-28.64005	34.01121
O	71.33631	-24.08781	31.08222
O	73.74984	-23.48202	32.19458
O	73.98044	-24.13740	35.03548
O	72.08798	-25.53251	36.11454
C*	67.23998	-22.83799	33.62699
C	69.72296	-22.26706	34.14577
C	68.51363	-22.06590	33.50869
N	70.57623	-21.29345	33.66835
N	68.63973	-20.98440	32.65997
C	69.88407	-20.55208	32.77763
C*	76.92097	-28.86699	39.93099
C	75.58073	-28.57072	39.31128
C	75.40791	-27.48600	38.43919
C	74.16479	-27.18583	37.87772
C	73.04784	-27.98484	38.18084
O	71.81194	-27.73919	37.69103
C	74.45692	-29.36639	39.59281
C	73.20871	-29.08761	39.03863
C*	77.29698	-23.20700	40.02999
C*	76.39197	-23.68199	38.88999
C*	75.38298	-22.57599	38.53599
C*	77.16697	-24.08299	37.64199
C	73.12757	-20.02482	31.84323
O	73.28936	-20.90561	32.95907
C*	72.55898	-20.73499	30.62099
C*	67.48798	-17.76800	29.31099
C	68.16275	-18.67277	30.31316
O	67.32346	-19.52824	30.87096
O	69.35393	-18.60209	30.57310
H	68.59707	-26.31137	32.59563
H	69.63857	-26.15500	31.15316
H	68.80271	-24.73374	31.76975
H	75.11089	-23.39959	30.68449
H	73.60204	-24.28096	30.26200
H	74.83331	-25.05011	31.33902
H	75.69455	-23.18454	35.51909
H	74.72349	-22.32398	34.28772
H	75.66373	-23.78987	33.83051
H	69.73052	-26.08587	36.10070
H	68.62897	-26.14520	34.72528
H	70.85811	-28.22964	35.32960
H	69.37111	-29.87161	34.53701
H	67.26103	-27.60486	34.10074
H	66.91591	-29.28785	34.55893
H	67.55208	-28.93370	32.94858
H	66.41628	-22.20218	33.99268
H	67.35491	-23.68236	34.32347
H	66.93008	-23.23849	32.64738
H	70.02514	-22.99601	34.89076
H	71.59509	-21.21192	33.78167
H	67.79146	-20.12503	31.56411
H	70.28757	-19.71822	32.20951
H	77.60295	-28.00780	39.83962
H	77.43297	-29.72633	39.46887
H	76.80540	-29.06875	41.00929
H	76.26303	-26.84961	38.19419
H	74.05053	-26.32735	37.21196
H	71.81400	-26.91639	37.15918
H	74.55663	-30.22366	40.26726

H	72.33604	-29.70451	39.26624
H	78.02075	-23.98561	40.32593
H	76.70670	-22.93674	40.92113
H	77.87412	-22.31507	39.72724
H	75.82701	-24.56492	39.24321
H	75.90722	-21.67821	38.16400
H	74.78548	-22.27583	39.41276
H	74.68105	-22.90662	37.75176
H	77.66203	-23.21036	37.18111
H	76.50168	-24.53591	36.89080
H	77.95275	-24.82431	37.86901
H	72.45710	-19.21511	32.17455
H	74.09517	-19.54880	31.59227
H	73.58947	-21.76583	32.60509
H	71.65910	-21.31335	30.87493
H	73.29360	-21.43680	30.19368
H	72.29014	-20.00265	29.84348
H	68.22397	-17.10024	28.84612
H	66.71009	-17.17536	29.81859
H	66.98298	-18.37249	28.54115
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05467	-36.07404	44.82532
N	80.36582	-36.51530	44.35990
C	81.51160	-36.38436	45.03509
N	81.50979	-36.14368	46.35570
N	82.66854	-36.48355	44.37270
C*	75.72200	-32.17300	44.73700
O	74.77134	-32.91892	44.66110
C*	81.64500	-32.53700	42.95900
N	79.55849	-31.16463	42.47315
C	80.31329	-32.32050	42.34390
C	78.34501	-31.34823	41.93832
N	78.30080	-32.59386	41.46782
C	79.50901	-33.20912	41.68236
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39906	-33.59912	39.57296
C*	77.25800	-32.00400	36.55700
O	77.92527	-31.14541	35.97576
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.13207	-36.54610	35.48473
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.81486	-36.66297	41.38511
N	72.80417	-35.20152	41.29471
C	73.02661	-34.39791	42.33368
N	73.02728	-34.88814	43.57675
N	73.22881	-33.08307	42.12866
C*	79.04600	-41.17200	35.58000
O	78.28523	-41.93564	34.99994
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17420	-43.77568	37.78011
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69677	-39.60993	40.66504
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62000	-39.32160	37.26668
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46058	-36.19515	41.25233
Fe	76.99105	-37.96920	39.84957
Fe	78.45186	-36.81682	37.61657
Fe	76.90021	-35.32955	39.46950
Fe	79.33901	-36.55004	40.36317
S	79.01079	-34.85009	38.72852
S	77.36455	-36.36888	41.54964

S	79.08775	-38.51789	39.07288
S	76.16498	-36.89353	37.91234
H	77.53261	-32.14054	45.86806
H	77.75923	-32.11722	44.13945
H	77.02648	-34.55640	45.89212
H	76.76184	-34.59693	44.14605
H	79.54005	-34.03167	45.39046
H	79.15646	-34.27052	43.67620
H	78.88261	-36.41154	45.86063
H	78.31408	-36.59719	44.20421
H	80.47260	-36.67006	43.34687
H	82.38243	-36.09464	46.86838
H	80.66601	-36.27201	46.90065
H	82.64637	-36.48929	43.34961
H	75.57592	-31.06727	44.65494
H	73.43625	-32.50958	42.94023
H	82.05769	-33.49198	42.60441
H	81.56007	-32.57797	44.05781
H	82.35351	-31.73421	42.70186
H	79.87108	-30.29617	42.90175
H	77.55514	-30.60685	41.88604
H	77.48160	-33.04865	41.04298
H	79.70514	-34.21725	41.34595
H	75.25617	-31.73537	37.31360
H	76.44486	-30.50664	37.76950
H	76.58785	-31.56562	39.74875
H	77.58152	-32.75503	38.92456
H	76.78230	-33.98446	36.69802
H	77.68914	-33.29055	34.12544
H	79.14558	-33.56931	35.08986
H	78.04087	-35.51016	33.65063
H	76.89989	-35.69987	34.99168
H	71.74619	-37.78230	38.21163
H	71.25047	-36.24619	38.95385
H	70.76574	-37.78820	39.70150
H	73.71527	-36.84620	39.44899
H	73.18309	-38.34308	40.16887
H	73.70771	-36.96829	41.95780
H	71.91910	-37.01341	41.93023
H	72.72925	-34.77303	40.37652
H	72.77592	-35.85063	43.76260
H	73.45585	-34.34648	44.32181
H	73.66055	-32.81556	41.24197
H	79.43602	-40.23677	35.11132
H	80.20189	-40.67634	37.15176
H	79.45499	-43.43751	37.02144
H	79.84065	-41.43963	39.36261
H	81.14757	-42.33578	38.53579
H	79.95456	-43.21316	39.52679
H	77.52740	-40.73110	38.46587
H	75.32101	-42.31816	39.43036
H	75.06573	-41.92116	37.71766
H	74.02337	-40.16819	39.02882
H	75.42665	-39.47104	38.22367
H	83.55944	-36.49702	44.85400
H	83.27378	-41.35655	37.03091
H	83.99764	-40.10795	36.01030
H	84.69920	-40.44180	37.62018
H	84.36242	-38.58358	38.61074
H	81.85109	-37.06427	38.31670
H	83.13109	-37.89858	40.99266
H	81.56754	-38.45718	40.37285
H	83.41599	-36.44832	38.92722

**Table S6.3 Ubiquinone stacked, SQ N2[ox]**

211

# E=-12375.76050826 Hartree

C	71.34034	-25.07689	32.89076
C	72.40805	-24.35274	32.21069
C	73.52599	-23.89958	33.02776
C	73.57114	-24.08294	34.39647
C	72.48711	-24.80238	35.06715
C	71.38115	-25.27775	34.26244
C	70.16150	-25.49794	32.05626
C	75.32693	-23.81462	31.44613
C	75.43821	-22.59937	34.89755
C	70.21521	-25.93086	34.98748
C	70.19862	-27.43595	34.88058
C	69.21017	-28.21133	34.40641
C	67.87692	-27.77431	33.86467
O	72.38298	-24.10687	30.97563
O	74.50160	-23.14703	32.39804
O	74.55538	-23.66479	35.23478
O	72.53273	-24.95590	36.33504
C*	67.23998	-22.83799	33.62699
C	69.74817	-22.31969	34.04642
C	68.50443	-22.04245	33.51546
N	70.58608	-21.31513	33.61511
N	68.59318	-20.87536	32.77637
C	69.85314	-20.47330	32.85789
C*	76.92097	-28.86699	39.93099
C	75.65052	-28.44942	39.24007
C	75.61970	-27.31689	38.41285
C	74.44281	-26.87695	37.80998
C	73.23656	-27.57960	38.01922
O	72.06855	-27.18085	37.50141
C	74.45099	-29.15884	39.41800
C	73.26330	-28.74162	38.81754
C*	77.29698	-23.20700	40.02999
C*	76.39197	-23.68199	38.88999
C*	75.38298	-22.57599	38.53599
C*	77.16697	-24.08299	37.64199
C	73.18500	-19.96279	31.77332
O	73.30190	-20.75653	32.95208
C*	72.55898	-20.73499	30.62099
C*	67.48798	-17.76800	29.31099
C	68.11676	-18.54074	30.44882
O	67.30861	-19.45734	30.94982
O	69.25257	-18.32473	30.84064
H	69.91046	-26.55864	32.20912
H	70.37472	-25.32184	30.99384
H	69.26388	-24.90969	32.32156
H	76.02684	-23.06261	31.05347
H	74.72056	-24.22483	30.62570
H	75.89916	-24.62354	31.93475
H	75.93242	-22.31488	35.83302
H	74.89466	-21.72934	34.50168
H	76.20043	-22.90900	34.16629
H	70.28135	-25.65846	36.05347
H	69.26970	-25.50834	34.61398
H	71.10705	-27.92084	35.25357
H	69.37783	-29.29679	34.40958
H	67.75440	-26.68160	33.85849
H	67.04912	-28.20296	34.45819
H	67.73522	-28.13215	32.82909
H	66.41028	-22.22792	34.02233
H	67.38138	-23.70053	34.29570
H	66.92425	-23.21930	32.64060
H	70.10106	-23.14154	34.65919
H	71.61261	-21.25637	33.67464
H	67.76105	-20.01324	31.69660
H	70.24130	-19.58989	32.35697
H	77.62085	-28.02226	40.03055
H	77.46740	-29.66917	39.40616
H	76.69157	-29.21546	40.95229
H	76.53942	-26.75093	38.24516
H	74.42651	-25.97511	37.19374
H	72.18094	-26.29196	37.02278



H	74.44084	-30.05302	40.05198
H	72.32929	-29.28866	38.96944
H	78.02502	-23.98321	40.32412
H	76.70777	-22.94014	40.92334
H	77.87066	-22.31215	39.72806
H	75.82380	-24.56259	39.24063
H	75.90693	-21.67595	38.16826
H	74.79042	-22.27669	39.41729
H	74.68272	-22.91407	37.75486
H	77.71816	-23.22078	37.22687
H	76.48926	-24.45925	36.86059
H	77.91193	-24.86884	37.85785
H	72.57307	-19.08358	32.03835
H	74.18101	-19.57635	31.47740
H	73.79668	-21.56313	32.69472
H	71.53191	-21.04580	30.85980
H	73.12331	-21.65668	30.41048
H	72.52763	-20.11318	29.71097
H	68.17778	-16.99397	28.95170
H	66.54365	-17.31068	29.64651
H	67.23906	-18.46056	28.49090
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05488	-36.07379	44.82526
N	80.36510	-36.51499	44.35654
C	81.51287	-36.37520	45.02633
N	81.51508	-36.12262	46.34487
N	82.66772	-36.48086	44.36119
C*	75.72200	-32.17300	44.73700
O	74.76936	-32.91822	44.68081
C*	81.64500	-32.53700	42.95900
N	79.57096	-31.15256	42.45875
C	80.31540	-32.31638	42.34148
C	78.35804	-31.32917	41.92098
N	78.30329	-32.57865	41.46206
C	79.50485	-33.20350	41.68600
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.40363	-33.60606	39.57017
C*	77.25800	-32.00400	36.55700
O	77.93348	-31.14878	35.98157
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.13150	-36.54774	35.48500
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.81740	-36.66392	41.38577
N	72.80783	-35.20268	41.29822
C	73.03758	-34.40149	42.33773
N	73.05839	-34.89786	43.57904
N	73.22629	-33.08531	42.13835
C*	79.04600	-41.17200	35.58000
O	78.28970	-41.93913	34.99840
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17463	-43.77621	37.78021
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69526	-39.61181	40.66621
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62072	-39.32128	37.26498
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46471	-36.19320	41.25203
Fe	76.99471	-37.97143	39.85120
Fe	78.45409	-36.81791	37.61752
Fe	76.90298	-35.33071	39.47089
Fe	79.34055	-36.54930	40.36424
S	79.01351	-34.85213	38.72914

S	77.36813	-36.37034	41.55174
S	79.09185	-38.52011	39.07481
S	76.16861	-36.89570	37.91524
H	77.53229	-32.14014	45.86804
H	77.75957	-32.11807	44.13864
H	77.02626	-34.55699	45.89184
H	76.76236	-34.59686	44.14560
H	79.54028	-34.03103	45.38980
H	79.15570	-34.27025	43.67613
H	78.88541	-36.41130	45.86122
H	78.31313	-36.59695	44.20560
H	80.46896	-36.67098	43.34316
H	82.38885	-36.06848	46.85481
H	80.67156	-36.24002	46.89257
H	82.64042	-36.48408	43.33751
H	75.57729	-31.06883	44.63728
H	73.42929	-32.50762	42.94769
H	82.04943	-33.49996	42.61676
H	81.56065	-32.56258	44.05838
H	82.36039	-31.74396	42.69066
H	79.89051	-30.28164	42.87713
H	77.57746	-30.57864	41.85463
H	77.48284	-33.02721	41.03327
H	79.69156	-34.21643	41.35925
H	75.25616	-31.73575	37.31353
H	76.44186	-30.50623	37.77100
H	76.57693	-31.56446	39.74823
H	77.58428	-32.74849	38.92835
H	76.76821	-33.98050	36.68656
H	77.68936	-33.29181	34.12455
H	79.14534	-33.56852	35.09005
H	78.04096	-35.51092	33.65077
H	76.90006	-35.70011	34.99188
H	71.74832	-37.77661	38.20900
H	71.24729	-36.24627	38.95880
H	70.76724	-37.79356	39.69865
H	73.71477	-36.84552	39.44886
H	73.18343	-38.34316	40.16804
H	73.71178	-36.97135	41.95511
H	71.92273	-37.01447	41.93297
H	72.71969	-34.77170	40.38235
H	72.82390	-35.86503	43.76149
H	73.49392	-34.35594	44.32011
H	73.62045	-32.79834	41.24150
H	79.43172	-40.23438	35.11278
H	80.19725	-40.67275	37.15447
H	79.45479	-43.43737	37.02111
H	79.84067	-41.43941	39.36221
H	81.14757	-42.33566	38.53578
H	79.95436	-43.21292	39.52713
H	77.52755	-40.73112	38.46752
H	75.32113	-42.31792	39.43068
H	75.06629	-41.92189	37.71757
H	74.02332	-40.16777	39.02686
H	75.42790	-39.47061	38.22451
H	83.56078	-36.46717	44.83825
H	83.26502	-41.35103	37.00477
H	84.02083	-40.09171	36.02003
H	84.68764	-40.46028	37.63666
H	84.36213	-38.58432	38.61166
H	81.85116	-37.06422	38.31666
H	83.13117	-37.90093	40.99160
H	81.56582	-38.45580	40.37250
H	83.41591	-36.44825	38.92732

**Table S6.4 Ubiquinone H-bonded, Q N2[red]**

211

# E=-12375.75002391 Hartree

C	72.05445	-24.74662	35.68251
C	71.94481	-23.99226	36.96824
C	72.17705	-22.52546	37.00894
C	72.63107	-21.88656	35.89418
C	72.83317	-22.65922	34.62387
C	72.52699	-24.11596	34.57693
C	71.65404	-26.19175	35.72825
C	70.71227	-21.77563	38.73007
C	73.03481	-19.66955	36.81955
C*	72.67300	-24.74800	33.21300
C	71.39464	-24.56275	32.42029
C	70.63011	-25.52270	31.87866
C	70.85230	-27.00745	31.89802
O	71.64276	-24.56532	38.01481
O	72.03891	-21.89782	38.19974
O	72.88962	-20.58695	35.72212
O	73.22156	-22.07831	33.62317
C*	67.24000	-22.83800	33.62700
C	69.40440	-21.77616	34.59210
C	68.41625	-21.91317	33.63872
N	70.25397	-20.79096	34.12095
N	68.67029	-21.02532	32.61029
C	69.77526	-20.37214	32.92879
C*	76.92100	-28.86700	39.93100
C	75.51038	-28.44788	39.60999
C	75.26249	-27.26346	38.90420
C	73.96415	-26.80740	38.66988
C	72.86045	-27.54722	39.12992
O	71.58161	-27.15198	38.93937
C	74.39856	-29.18949	40.04568
C	73.09325	-28.75566	39.81061
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.05747	-19.50406	31.37601
O	74.13838	-19.76936	32.25002
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.19917	-18.77017	30.19040
O	67.37912	-19.68128	30.69098
O	69.39640	-18.72305	30.42331
H	71.43196	-26.58425	34.72964
H	70.76906	-26.33141	36.36434
H	72.46126	-26.80381	36.16649
H	70.81194	-21.25433	39.69096
H	70.25258	-22.76119	38.89355
H	70.08028	-21.17313	38.05359
H	73.40753	-18.74197	36.36776
H	73.75744	-20.05666	37.55052
H	72.06939	-19.48837	37.31315
H	73.49886	-24.24420	32.68734
H	72.94044	-25.80753	33.30927
H	71.07226	-23.52133	32.30701
H	69.72918	-25.19266	31.34551
H	71.78591	-27.30259	32.39948
H	70.88400	-27.40884	30.87003
H	70.01565	-27.52059	32.40479
H	66.29653	-22.27670	33.52478
H	67.19475	-23.42891	34.55346
H	67.29934	-23.53683	32.77559
H	69.56949	-22.28729	35.53588
H	71.09472	-20.43499	34.56874
H	67.86162	-20.28613	31.35779
H	70.22818	-19.59705	32.31499
H	77.64451	-28.43470	39.22258
H	77.04457	-29.95244	39.88547
H	77.21895	-28.52619	40.94016
H	76.10494	-26.67750	38.52846
H	73.80595	-25.86735	38.14001
H	71.55924	-26.24652	38.56390

H	74.55330	-30.13202	40.58173
H	72.23353	-29.33672	40.15303
H	78.01251	-23.99018	40.33335
H	76.70539	-22.92703	40.91742
H	77.88269	-22.32209	39.72344
H	75.82204	-24.55680	39.24898
H	75.90835	-21.65431	38.22831
H	74.72168	-22.32726	39.38108
H	74.73976	-22.88032	37.69588
H	77.72045	-23.22191	37.22800
H	76.49111	-24.45454	36.85354
H	77.90264	-24.87815	37.85265
H	72.21090	-19.03360	31.91892
H	73.41026	-18.74476	30.65663
H	73.84686	-20.44528	32.88398
H	72.19854	-21.50361	31.32322
H	73.37143	-21.17781	30.02234
H	71.72307	-20.46238	29.95647
H	68.21511	-17.09412	28.84116
H	66.78240	-17.18628	29.92610
H	66.89643	-18.28988	28.54293
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.04078	-36.07810	44.79538
N	80.34779	-36.51957	44.32107
C	81.49496	-36.38243	44.98969
N	81.49565	-36.14637	46.31441
N	82.64842	-36.46892	44.32100
C*	75.72200	-32.17300	44.73700
O	74.77363	-32.92080	44.65166
C*	81.64500	-32.53700	42.95900
N	79.57074	-31.17276	42.38738
C	80.31206	-32.34375	42.33972
C	78.35746	-31.37973	41.85789
N	78.30156	-32.65457	41.47372
C	79.49882	-33.26598	41.73914
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39317	-33.60687	39.52743
C*	77.25800	-32.00400	36.55700
O	77.90011	-31.13807	35.95355
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.19616	-36.53023	35.39582
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.83581	-36.62237	41.36622
N	72.86355	-35.16258	41.23322
C	73.03488	-34.33434	42.26240
N	72.87200	-34.77236	43.51724
N	73.33714	-33.04294	42.03470
C*	79.04600	-41.17200	35.58000
O	78.32183	-41.96021	34.98280
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17251	-43.77566	37.76710
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.63326	-39.62817	40.69182
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62623	-39.31806	37.25170
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.47645	-36.20851	41.27309
Fe	76.98514	-37.95817	39.91157
Fe	78.45840	-36.92811	37.52944
Fe	76.91049	-35.37971	39.47370
Fe	79.33014	-36.50068	40.39498
S	79.01238	-34.84687	38.76460

S	77.29621	-36.32670	41.61393
S	79.07395	-38.57071	39.23546
S	76.11895	-36.94570	37.95494
H	77.53757	-32.13620	45.86402
H	77.75513	-32.12025	44.13254
H	77.02421	-34.55751	45.89115
H	76.76697	-34.59530	44.14145
H	79.54040	-34.04756	45.40251
H	79.15892	-34.25659	43.68376
H	78.86328	-36.43672	45.82344
H	78.29854	-36.57549	44.15517
H	80.45190	-36.65830	43.30122
H	82.36964	-36.11377	46.82518
H	80.65415	-36.29385	46.85790
H	82.60535	-36.45380	43.29193
H	75.57529	-31.06598	44.66223
H	73.52824	-32.46643	42.84759
H	82.04160	-33.51748	42.65842
H	81.57047	-32.51154	44.05945
H	82.36276	-31.76177	42.64794
H	79.89243	-30.28020	42.75366
H	77.57928	-30.63294	41.75343
H	77.49330	-33.13668	41.05425
H	79.67827	-34.30104	41.48336
H	75.25746	-31.73960	37.31203
H	76.44979	-30.50488	37.77137
H	76.57539	-31.58158	39.76141
H	77.57925	-32.76570	38.92892
H	76.87147	-34.00459	36.76326
H	77.69075	-33.27608	34.13324
H	79.14756	-33.57466	35.09103
H	77.94864	-35.49458	33.64177
H	76.92222	-35.70452	35.06650
H	71.73751	-37.81403	38.22750
H	71.27155	-36.24620	38.92393
H	70.75429	-37.75621	39.71482
H	73.72635	-36.88746	39.43387
H	73.16740	-38.34264	40.19987
H	73.72076	-36.93944	41.94556
H	71.92820	-36.92613	41.91950
H	72.98426	-34.77252	40.30162
H	72.61756	-35.73451	43.70049
H	73.27956	-34.23547	44.27676
H	73.88442	-32.85641	41.18280
H	79.40144	-40.21593	35.12688
H	80.14969	-40.63900	37.18255
H	79.45403	-43.43565	37.01816
H	79.84366	-41.43530	39.35657
H	81.14771	-42.33976	38.53531
H	79.95057	-43.21086	39.52941
H	77.53564	-40.73809	38.51824
H	75.31847	-42.32051	39.42827
H	75.07270	-41.92419	37.71422
H	74.02290	-40.15845	38.97760
H	75.46627	-39.46342	38.24743
H	83.54191	-36.45843	44.79657
H	83.25655	-41.34521	36.98101
H	84.04129	-40.07710	36.02945
H	84.67754	-40.47928	37.65021
H	84.35687	-38.59610	38.62866
H	81.84806	-37.06661	38.31978
H	83.13222	-37.92661	40.97931
H	81.54702	-38.43989	40.35811
H	83.41697	-36.44831	38.92386

Table S6.5 Ubiquinone H-bonded, Q N2[ox]

211

# E=-12375.61575879 Hartree			
C	72.06948	-24.82062	35.67262
C	71.88888	-24.10814	36.97019
C	72.06221	-22.61674	37.03362
C	72.49275	-21.95389	35.91834
C	72.76477	-22.66721	34.66322
C	72.51955	-24.14122	34.58545
C	71.73525	-26.28724	35.62764
C	71.19026	-22.37896	39.31970
C	73.84451	-19.97616	35.89062
C*	72.67300	-24.74800	33.21300
C	71.41399	-24.47145	32.41184
C	70.54273	-25.37099	31.93045
C	70.59874	-26.86790	32.02952
O	71.60585	-24.71580	37.99929
O	71.86311	-21.91101	38.14113
O	72.54836	-20.59819	35.90431
O	73.15662	-22.05571	33.67220
C*	67.24000	-22.83800	33.62700
C	69.27015	-21.73492	34.79143
C	68.22655	-21.74368	33.88959
N	69.88410	-20.50499	34.65794
N	68.21746	-20.53499	33.21514
C	69.22460	-19.82281	33.69879
C*	76.92100	-28.86700	39.93100
C	75.49652	-28.50019	39.61379
C	75.21037	-27.35319	38.86046
C	73.89892	-26.93101	38.64192
C	72.82300	-27.66212	39.17432
O	71.53169	-27.28641	39.01736
C	74.41086	-29.24182	40.10966
C	73.09209	-28.83821	39.89555
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	71.55342	-20.16212	31.61157
O	72.17249	-19.59073	32.75505
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	67.92841	-18.38169	30.62361
O	67.22979	-19.45747	30.95117
O	68.83943	-17.92710	31.29677
H	70.95371	-26.47559	34.87523
H	71.37903	-26.65980	36.59293
H	72.61591	-26.88406	35.33985
H	71.01546	-21.47601	39.91886
H	71.81719	-23.08847	39.87629
H	70.23146	-22.85582	39.07152
H	73.67022	-18.90585	35.72373
H	74.46567	-20.37641	35.07482
H	74.34613	-20.12819	36.85977
H	73.52845	-24.26744	32.71311
H	72.88022	-25.82253	33.28345
H	71.20827	-23.40830	32.24513
H	69.67842	-24.97285	31.38347
H	71.49684	-27.23770	32.54556
H	70.57454	-27.32441	31.02462
H	69.71366	-27.25529	32.56506
H	66.20646	-22.49772	33.80710
H	67.43733	-23.70455	34.27507
H	67.29358	-23.17486	32.57778
H	69.60835	-22.48504	35.49919
H	70.75500	-20.20789	35.09888
H	67.56412	-19.87251	31.82514
H	69.52450	-18.84481	33.33113
H	77.62489	-28.41229	39.21713
H	77.09471	-29.94754	39.90174
H	77.20939	-28.50407	40.93522
H	76.03198	-26.76826	38.43851
H	73.70890	-26.02519	38.06654

H	71.48847	-26.38818	38.63006
H	74.59835	-30.15445	40.68619
H	72.25087	-29.41338	40.28980
H	78.01709	-23.98792	40.32821
H	76.70680	-22.93272	40.92003
H	77.87751	-22.31834	39.72499
H	75.82266	-24.55985	39.24692
H	75.90852	-21.66205	38.20776
H	74.74481	-22.30738	39.39358
H	74.72098	-22.88514	37.71119
H	77.72457	-23.22313	37.23117
H	76.49111	-24.44906	36.85077
H	77.89919	-24.88164	37.85192
H	70.83248	-20.95327	31.90326
H	70.95486	-19.36219	31.14775
H	72.63953	-20.31228	33.20979
H	73.12639	-21.56045	31.08161
H	73.27572	-19.95950	30.30441
H	72.04977	-21.12738	29.72447
H	68.05361	-16.84804	29.11820
H	66.40807	-17.55458	29.34044
H	67.65537	-18.49000	28.49555
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05733	-36.07308	44.83252
N	80.36742	-36.51456	44.36447
C	81.51431	-36.38992	45.03920
N	81.51459	-36.15450	46.36088
N	82.67018	-36.48955	44.37526
C*	75.72200	-32.17300	44.73700
O	74.77238	-32.91856	44.64787
C*	81.64500	-32.53700	42.95900
N	79.56217	-31.14046	42.53261
C	80.30841	-32.29660	42.36154
C	78.34251	-31.29820	42.00340
N	78.28666	-32.52878	41.49317
C	79.49265	-33.15945	41.67913
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39840	-33.60142	39.57071
C*	77.25800	-32.00400	36.55700
O	77.92195	-31.14479	35.97332
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.13040	-36.54440	35.49013
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.81632	-36.65640	41.38208
N	72.79977	-35.19511	41.28591
C	73.01545	-34.38784	42.32332
N	73.01927	-34.87628	43.56712
N	73.20626	-33.07097	42.11726
C*	79.04600	-41.17200	35.58000
O	78.28492	-41.93543	35.00013
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17419	-43.77566	37.78028
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.70029	-39.60869	40.66357
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.61993	-39.32161	37.26684
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46733	-36.19122	41.25535
Fe	76.99738	-37.96509	39.85656
Fe	78.45491	-36.80999	37.62409
Fe	76.90813	-35.32380	39.48482
Fe	79.34402	-36.54177	40.37370

S	79.01568	-34.84261	38.73692
S	77.37011	-36.36807	41.56113
S	79.09332	-38.51024	39.07886
S	76.16979	-36.88646	37.92362
H	77.53220	-32.14091	45.86838
H	77.75945	-32.11730	44.14091
H	77.02689	-34.55570	45.89259
H	76.76170	-34.59737	44.14652
H	79.54099	-34.02718	45.38615
H	79.15403	-34.27601	43.67329
H	78.88968	-36.40518	45.87020
H	78.31501	-36.60037	44.21702
H	80.47282	-36.66590	43.35081
H	82.38805	-36.11149	46.87269
H	80.67150	-36.28508	46.90644
H	82.64688	-36.49249	43.35203
H	75.57511	-31.06638	44.66671
H	73.41573	-32.49654	42.92759
H	82.05318	-33.47953	42.56777
H	81.56687	-32.61753	44.05614
H	82.35268	-31.72628	42.72587
H	79.88424	-30.28950	42.98866
H	77.55547	-30.55139	41.99039
H	77.46247	-32.96872	41.06288
H	79.67692	-34.15851	41.30839
H	75.25593	-31.73475	37.31390
H	76.45195	-30.50644	37.77703
H	76.57399	-31.57348	39.75352
H	77.58433	-32.74915	38.93024
H	76.78887	-33.98632	36.70323
H	77.68898	-33.29035	34.12568
H	79.14565	-33.56951	35.08971
H	78.04455	-35.51080	33.65114
H	76.89910	-35.69954	34.98891
H	71.74372	-37.78984	38.21525
H	71.25523	-36.24626	38.94641
H	70.76331	-37.78059	39.70507
H	73.71657	-36.85117	39.44694
H	73.18017	-38.34314	40.17419
H	73.71174	-36.95637	41.95363
H	71.92321	-37.00726	41.93118
H	72.72391	-34.77045	40.36604
H	72.78329	-35.84277	43.75233
H	73.44642	-34.33184	44.31093
H	73.62515	-32.79815	41.22643
H	79.43638	-40.23700	35.11114
H	80.20219	-40.67655	37.15161
H	79.45502	-43.43753	37.02148
H	79.84094	-41.43938	39.36237
H	81.14758	-42.33621	38.53581
H	79.95426	-43.21294	39.52700
H	77.52723	-40.73100	38.46544
H	75.32100	-42.31814	39.43037
H	75.06559	-41.92110	37.71772
H	74.02343	-40.16857	39.03124
H	75.42570	-39.47066	38.22360
H	83.56139	-36.51040	44.85577
H	83.27303	-41.35611	37.02885
H	83.99948	-40.10670	36.01102
H	84.69831	-40.44329	37.62147
H	84.36246	-38.58346	38.61064
H	81.85122	-37.06398	38.31667
H	83.13061	-37.90193	40.99164
H	81.56415	-38.45433	40.37331
H	83.41622	-36.44851	38.92747



**Table S6.6 Ubiquinone H-bonded, SQ N2[ox]**

211

# E=-12375.76354084 Hartree

C	72.12343	-24.78154	35.70135
C	71.98101	-24.08606	36.97033
C	72.25112	-22.65486	37.01167
C	72.70468	-21.98473	35.89007
C	72.91555	-22.69950	34.63333
C	72.59227	-24.10883	34.58572
C	71.73375	-26.23695	35.62591
C	70.86469	-21.91599	38.80415
C	72.43898	-19.69733	36.68573
C*	72.67300	-24.74800	33.21300
C	71.36439	-24.58717	32.47411
C	70.57110	-25.54894	31.97674
C	70.79449	-27.03560	32.00317
O	71.63317	-24.67298	38.04882
O	72.15715	-22.00233	38.21478
O	72.96428	-20.65465	35.77537
O	73.27949	-22.07570	33.59275
C*	67.24000	-22.83800	33.62700
C	69.60851	-22.04071	34.33380
C	68.46000	-21.97342	33.57195
N	70.43431	-21.03849	33.86397
N	68.60022	-20.94818	32.65394
C	69.79623	-20.41650	32.85308
C*	76.92100	-28.86700	39.93100
C	75.51214	-28.43905	39.61276
C	75.26957	-27.29583	38.83520
C	73.97860	-26.81880	38.61121
C	72.86715	-27.48914	39.16295
O	71.60739	-27.06079	38.99863
C	74.39742	-29.11709	40.13354
C	73.09669	-28.66011	39.91422
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.10346	-19.57847	31.46126
O	74.22148	-19.92296	32.24698
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.16405	-18.76086	30.22499
O	67.30502	-19.55204	30.84103
O	69.37524	-18.79605	30.37768
H	70.97724	-26.39875	34.84104
H	71.32787	-26.59356	36.57865
H	72.59851	-26.87508	35.37342
H	70.97212	-21.30493	39.71266
H	70.47844	-22.91105	39.07028
H	70.14991	-21.41674	38.12258
H	72.63216	-18.71627	36.22802
H	72.92562	-19.75450	37.66918
H	71.35009	-19.82450	36.81575
H	73.45827	-24.22539	32.64423
H	72.96023	-25.80609	33.28766
H	71.03590	-23.54765	32.36792
H	69.64388	-25.22541	31.48514
H	71.72365	-27.32010	32.51843
H	70.83787	-27.44668	30.97828
H	69.95769	-27.55084	32.50842
H	66.33086	-22.24038	33.80953
H	67.32883	-23.58697	34.42774
H	67.09448	-23.37235	32.67287
H	69.91600	-22.71693	35.12638
H	71.40548	-20.87471	34.12496
H	67.77749	-20.17128	31.52331
H	70.21416	-19.60682	32.26113
H	77.64035	-28.47368	39.19580
H	77.03787	-29.95557	39.93577
H	77.24160	-28.48815	40.92043
H	76.11424	-26.75546	38.39855
H	73.81644	-25.91614	38.02109
H	71.59787	-26.14826	38.56101

H	74.54887	-30.02040	40.73679
H	72.23350	-29.18836	40.32750
H	78.01527	-23.98788	40.33563
H	76.70429	-22.92643	40.91677
H	77.88033	-22.32038	39.72319
H	75.82347	-24.56001	39.24561
H	75.90927	-21.65077	38.24073
H	74.71356	-22.33569	39.37639
H	74.74189	-22.87282	37.69339
H	77.72047	-23.22169	37.22789
H	76.48810	-24.44975	36.85433
H	77.90246	-24.87986	37.85083
H	72.28422	-19.16478	32.08920
H	73.41248	-18.75077	30.79677
H	73.93552	-20.62872	32.86673
H	72.26752	-21.57056	31.27690
H	73.33200	-21.10210	29.92545
H	71.67482	-20.41321	30.04590
H	68.23788	-17.19612	28.75001
H	66.87183	-17.08223	29.91522
H	66.80830	-18.28981	28.61926
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05754	-36.07282	44.83261
N	80.36795	-36.51355	44.36416
C	81.51598	-36.37220	45.03349
N	81.51857	-36.11935	46.35196
N	82.67057	-36.47650	44.36781
C*	75.72200	-32.17300	44.73700
O	74.77172	-32.91909	44.66029
C*	81.64500	-32.53700	42.95900
N	79.57133	-31.12935	42.52322
C	80.30892	-32.29280	42.36220
C	78.35405	-31.27895	41.98691
N	78.29091	-32.51199	41.48339
C	79.48979	-33.15253	41.68041
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.40113	-33.61233	39.55544
C*	77.25800	-32.00400	36.55700
O	77.92785	-31.14778	35.97675
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.13140	-36.54627	35.48780
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.82184	-36.65313	41.38069
N	72.80734	-35.19248	41.28202
C	73.02275	-34.38376	42.31885
N	73.03124	-34.87320	43.56316
N	73.20737	-33.06772	42.11457
C*	79.04600	-41.17200	35.58000
O	78.28972	-41.93910	34.99833
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17452	-43.77612	37.78003
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69807	-39.61072	40.66506
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62039	-39.32247	37.26596
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46856	-36.19176	41.25612
Fe	77.00024	-37.96852	39.85647
Fe	78.45931	-36.81401	37.62311
Fe	76.90992	-35.32688	39.48035
Fe	79.34383	-36.54144	40.37300
S	79.01830	-34.84622	38.73447

S	77.37076	-36.36834	41.55925
S	79.09749	-38.51425	39.08149
S	76.17520	-36.89319	37.92153
H	77.53272	-32.14029	45.86785
H	77.75936	-32.11835	44.13956
H	77.02661	-34.55636	45.89228
H	76.76203	-34.59712	44.14615
H	79.54119	-34.02639	45.38540
H	79.15354	-34.27597	43.67322
H	78.89067	-36.40577	45.87035
H	78.31566	-36.60044	44.21684
H	80.47148	-36.66975	43.35098
H	82.39253	-36.06463	46.86152
H	80.67545	-36.23726	46.90021
H	82.64327	-36.48120	43.34410
H	75.57577	-31.06725	44.65609
H	73.40339	-32.48481	42.92173
H	82.02472	-33.50912	42.61481
H	81.58008	-32.55297	44.05971
H	82.37049	-31.75959	42.67199
H	79.89753	-30.27702	42.97390
H	77.57540	-30.52342	41.96036
H	77.46793	-32.94440	41.04439
H	79.66760	-34.15522	41.31674
H	75.25552	-31.73264	37.31454
H	76.45181	-30.50654	37.77916
H	76.55646	-31.57553	39.75510
H	77.58789	-32.74046	38.93520
H	76.77729	-33.98302	36.69420
H	77.68926	-33.29123	34.12497
H	79.14549	-33.56891	35.08972
H	78.04273	-35.51142	33.65105
H	76.89979	-35.69997	34.99108
H	71.74257	-37.79468	38.21767
H	71.25863	-36.24638	38.94148
H	70.76149	-37.77553	39.70719
H	73.71645	-36.85392	39.44444
H	73.17919	-38.34322	40.17585
H	73.71927	-36.95431	41.94874
H	71.93021	-37.00180	41.93380
H	72.73402	-34.76927	40.36127
H	72.81159	-35.84399	43.74543
H	73.46055	-34.32753	44.30487
H	73.59522	-32.78055	41.21513
H	79.43158	-40.23423	35.11295
H	80.19759	-40.67298	37.15437
H	79.45491	-43.43741	37.02123
H	79.84099	-41.43927	39.36215
H	81.14758	-42.33605	38.53573
H	79.95415	-43.21290	39.52710
H	77.52754	-40.73117	38.46807
H	75.32108	-42.31819	39.43041
H	75.06625	-41.92152	37.71745
H	74.02335	-40.16788	39.02849
H	75.42754	-39.47047	38.22450
H	83.56368	-36.46259	44.84478
H	83.27582	-41.35775	37.03751
H	83.99166	-40.11203	36.00795
H	84.70223	-40.43740	37.61573
H	84.36232	-38.58366	38.61091
H	81.85120	-37.06401	38.31671
H	83.13092	-37.90312	40.99079
H	81.56363	-38.45390	40.37257
H	83.41610	-36.44842	38.92725

**Table S6.7 Menaquinone stacked, Q N2[red]**

209

# E=-12300.35116828 Hartree

C	71.10832	-25.20052	32.73621
C	72.17450	-24.59473	31.87193
C	73.44774	-24.16257	32.51561
C	73.59067	-24.22932	33.91251
C	72.51331	-24.82718	34.74408
C	71.27429	-25.31419	34.08537
C	69.84857	-25.62618	32.04492
C*	70.21510	-25.92740	34.97980
C	70.26910	-27.43885	34.97239
C	69.27516	-28.27833	34.64374
C	67.87769	-27.93727	34.21202
O	72.00128	-24.44671	30.67198
O	72.65839	-24.91114	35.96549
C*	67.24000	-22.83800	33.62700
C	69.72396	-22.28521	34.15034
C	68.51509	-22.06780	33.51903
N	70.58310	-21.31397	33.67888
N	68.64450	-20.97583	32.68342
C	69.89185	-20.55333	32.80303
C*	76.92100	-28.86700	39.93100
C	75.64639	-28.41028	39.27145
C	75.64218	-27.30590	38.40940
C	74.46374	-26.83169	37.83156
C	73.24120	-27.46662	38.10618
O	72.06392	-27.02929	37.60396
C	74.42039	-29.05427	39.51312
C	73.23270	-28.59669	38.94240
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.11256	-19.95665	31.80886
O	73.27663	-20.75043	32.98981
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.16298	-18.65716	30.32960
O	67.32747	-19.51707	30.88682
O	69.35064	-18.57273	30.60094
H	69.59019	-26.66283	32.30730
H	69.94857	-25.53726	30.95685
H	69.00877	-24.98568	32.36709
H	70.36410	-25.56507	36.00852
H	69.22512	-25.57027	34.66255
H	71.22655	-27.86213	35.29131
H	69.49347	-29.35220	34.70590
H	67.69369	-26.85497	34.14724
H	67.13996	-28.36204	34.91541
H	67.65415	-28.37875	33.22474
H	66.40920	-22.19634	33.96524
H	67.34048	-23.66980	34.34082
H	66.94880	-23.25667	32.64878
H	70.02388	-23.02356	34.88739
H	71.59735	-21.22613	33.80804
H	67.79617	-20.10774	31.58440
H	70.29763	-19.71086	32.24948
H	77.69287	-28.08301	39.89018
H	77.35433	-29.76208	39.46048
H	76.74051	-29.08756	40.99699
H	76.58140	-26.79286	38.19043
H	74.47988	-25.95704	37.17903
H	72.20647	-26.22206	37.06631
H	74.38887	-29.92905	40.17130
H	72.28007	-29.09295	39.14255
H	78.02354	-23.98452	40.32166
H	76.70644	-22.94349	40.92295
H	77.87076	-22.31146	39.73096
H	75.82722	-24.56335	39.24378
H	75.90279	-21.68620	38.13973
H	74.80109	-22.26069	39.41789
H	74.66237	-22.91435	37.77205
H	77.67876	-23.21145	37.19687

H	76.50248	-24.50908	36.87395
H	77.93959	-24.83925	37.86125
H	72.42553	-19.14368	32.09158
H	74.07264	-19.47675	31.53999
H	73.94039	-21.43214	32.81335
H	71.63906	-21.27423	30.88966
H	73.28762	-21.47432	30.25298
H	72.32081	-20.04564	29.79545
H	68.22057	-17.09116	28.85393
H	66.69215	-17.18588	29.80253
H	67.00612	-18.38587	28.53693
H	74.84907	-23.79848	35.60283
C	74.76429	-23.75976	34.51724
C	75.80388	-23.25599	33.73264
H	76.71875	-22.89383	34.20757
C	75.67555	-23.22305	32.33588
H	76.49371	-22.84128	31.72040
C	74.49734	-23.67086	31.72932
H	74.37281	-23.64395	30.64564
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.03828	-36.07830	44.79720
N	80.34101	-36.52489	44.31672
C	81.49204	-36.39816	44.98092
N	81.50070	-36.16487	46.30606
N	82.64166	-36.49351	44.30694
C*	75.72200	-32.17300	44.73700
O	74.77206	-32.91991	44.66206
C*	81.64500	-32.53700	42.95900
N	79.54221	-31.20379	42.40026
C	80.31392	-32.35469	42.33024
C	78.33217	-31.43495	41.87125
N	78.30941	-32.70264	41.46424
C	79.52434	-33.28553	41.71259
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39326	-33.60418	39.53401
C*	77.25800	-32.00400	36.55700
O	77.90280	-31.13843	35.95554
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.19687	-36.53209	35.39110
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.83335	-36.63112	41.36997
N	72.86295	-35.17117	41.24507
C	73.04630	-34.34924	42.27675
N	72.89993	-34.79527	43.53087
N	73.34490	-33.05634	42.05221
C*	79.04600	-41.17200	35.58000
O	78.32167	-41.96008	34.98283
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17262	-43.77576	37.76729
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.63263	-39.62824	40.69187
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62628	-39.31792	37.25161
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.47123	-36.20975	41.26828
Fe	76.98127	-37.95928	39.90545
Fe	78.45464	-36.93301	37.52238
Fe	76.90450	-35.38285	39.46360
Fe	79.32604	-36.50535	40.38479
S	79.00773	-34.85298	38.75363
S	77.29440	-36.32774	41.60648
S	79.06972	-38.57496	39.22870

S	76.11439	-36.94923	37.94702
H	77.53443	-32.13771	45.86619
H	77.75711	-32.11884	44.13576
H	77.02402	-34.55763	45.89101
H	76.76722	-34.59539	44.14124
H	79.54113	-34.04726	45.40152
H	79.15899	-34.25829	43.68251
H	78.86535	-36.43438	45.82689
H	78.29086	-36.57482	44.16222
H	80.43983	-36.66152	43.29631
H	82.37748	-36.13823	46.81234
H	80.66062	-36.30470	46.85359
H	82.59321	-36.47111	43.27798
H	75.57612	-31.06661	44.65352
H	73.54028	-32.48395	42.86712
H	82.05029	-33.51457	42.66065
H	81.56272	-32.51140	44.05872
H	82.35938	-31.75657	42.65256
H	79.83951	-30.30998	42.78342
H	77.53191	-30.70935	41.77961
H	77.50795	-33.19896	41.04742
H	79.73495	-34.30951	41.43715
H	75.25823	-31.74374	37.31097
H	76.44087	-30.50428	37.76317
H	76.58593	-31.57226	39.75555
H	77.57732	-32.76959	38.92605
H	76.86678	-34.00371	36.76002
H	77.69088	-33.27628	34.13304
H	79.14753	-33.57453	35.09118
H	77.94520	-35.49414	33.64163
H	76.92306	-35.70463	35.06892
H	71.74053	-37.80539	38.22311
H	71.26593	-36.24594	38.93212
H	70.75687	-37.76503	39.71077
H	73.72485	-36.88087	39.43654
H	73.17090	-38.34283	40.19311
H	73.71740	-36.95207	41.94851
H	71.92465	-36.93748	41.92022
H	72.96657	-34.77468	40.31421
H	72.64636	-35.75818	43.71147
H	73.31889	-34.26327	44.28775
H	73.89423	-32.86786	41.20176
H	79.40156	-40.21597	35.12686
H	80.14962	-40.63898	37.18256
H	79.45405	-43.43564	37.01815
H	79.84321	-41.43561	39.35688
H	81.14769	-42.33919	38.53528
H	79.95100	-43.21117	39.52912
H	77.53555	-40.73792	38.51759
H	75.31850	-42.32049	39.42830
H	75.07266	-41.92425	37.71426
H	74.02289	-40.15876	38.97750
H	75.46570	-39.46376	38.24692
H	83.53748	-36.48740	44.77826
H	83.25555	-41.34440	36.97751
H	84.04443	-40.07502	36.03091
H	84.67586	-40.48173	37.65237
H	84.35689	-38.59610	38.62857
H	81.84786	-37.06684	38.31996
H	83.13247	-37.92347	40.98072
H	81.54934	-38.44194	40.35815
H	83.41676	-36.44815	38.92377

**Table S6.8 Menaquinone stacked, Q N2[ox]**

209

# E=-12300.21507236 Hartree			
C	71.11080	-25.19774	32.73859
C	72.17971	-24.59465	31.87528
C	73.45129	-24.16116	32.52138
C	73.59248	-24.22927	33.91848
C	72.51529	-24.83053	34.74737
C	71.27585	-25.31297	34.08783
C	69.85063	-25.62061	32.04692
C*	70.21510	-25.92740	34.97980
C	70.26870	-27.43882	34.96668
C	69.27482	-28.27851	34.63848
C	67.87516	-27.93950	34.21284
O	72.00976	-24.45092	30.67463
O	72.66262	-24.92345	35.96853
C*	67.24000	-22.83800	33.62700
C	69.72339	-22.28407	34.15433
C	68.51586	-22.06922	33.51937
N	70.58289	-21.31337	33.68214
N	68.64654	-20.97999	32.68089
C	69.89301	-20.55589	32.80230
C*	76.92100	-28.86700	39.93100
C	75.65145	-28.41885	39.25614
C	75.64907	-27.32149	38.38521
C	74.47070	-26.84967	37.80533
C	73.24675	-27.47945	38.08677
O	72.07012	-27.04307	37.58817
C	74.42452	-29.05942	39.50335
C	73.23749	-28.60556	38.92977
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.11131	-19.95484	31.80810
O	73.27498	-20.74715	32.99058
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.16422	-18.66164	30.32438
O	67.32889	-19.52389	30.87909
O	69.35209	-18.57941	30.59549
H	69.59182	-26.65781	32.30685
H	69.94915	-25.52876	30.95901
H	69.01173	-24.98054	32.37223
H	70.36277	-25.56816	36.00983
H	69.22567	-25.56859	34.66284
H	71.22800	-27.86300	35.27896
H	69.49575	-29.35226	34.69530
H	67.68809	-26.85760	34.15134
H	67.14107	-28.36793	34.91781
H	67.64929	-28.37935	33.22540
H	66.41069	-22.19637	33.96888
H	67.34025	-23.67240	34.33790
H	66.94638	-23.25245	32.64777
H	70.02173	-23.01942	34.89509
H	71.59661	-21.22392	33.81330
H	67.79744	-20.11341	31.57603
H	70.29908	-19.71429	32.24755
H	77.73438	-28.14238	39.77278
H	77.28951	-29.83488	39.56256
H	76.76460	-28.94275	41.02186
H	76.58834	-26.81048	38.16182
H	74.48726	-25.97952	37.14702
H	72.20840	-26.23257	37.05210
H	74.39210	-29.92620	40.17254
H	72.28350	-29.09710	39.13475
H	78.01972	-23.98656	40.32604
H	76.70608	-22.93711	40.92074
H	77.87526	-22.31531	39.72856
H	75.82689	-24.56360	39.24359
H	75.90298	-21.68523	38.14245
H	74.79937	-22.26262	39.41734
H	74.66399	-22.91336	37.77016

H	77.68188	-23.21221	37.19923
H	76.50214	-24.50511	36.87208
H	77.93752	-24.84176	37.86071
H	72.42388	-19.14164	32.08898
H	74.07146	-19.47514	31.53956
H	73.94648	-21.42213	32.81840
H	71.63618	-21.27018	30.88782
H	73.28659	-21.47745	30.25716
H	72.32582	-20.04716	29.79279
H	68.21985	-17.08989	28.85471
H	66.69418	-17.18718	29.80732
H	67.00317	-18.38207	28.53579
H	74.84786	-23.79711	35.61071
C	74.76481	-23.75868	34.52497
C	75.80471	-23.25268	33.74225
H	76.71816	-22.88873	34.21858
C	75.67825	-23.21874	32.34533
H	76.49631	-22.83460	31.73125
C	74.50131	-23.66754	31.73693
H	74.37807	-23.63926	30.65317
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05830	-36.07288	44.83295
N	80.36962	-36.51286	44.36631
C	81.51681	-36.37310	45.03763
N	81.51749	-36.12120	46.35616
N	82.67231	-36.47535	44.37332
C*	75.72200	-32.17300	44.73700
O	74.76940	-32.91806	44.67650
C*	81.64500	-32.53700	42.95900
N	79.60753	-31.11255	42.43604
C	80.31450	-32.30177	42.34800
C	78.38737	-31.26318	41.90787
N	78.29089	-32.52299	41.48217
C	79.47209	-33.18080	41.72093
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39662	-33.59706	39.57720
C*	77.25800	-32.00400	36.55700
O	77.92282	-31.14488	35.97407
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.12821	-36.54370	35.49450
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.81521	-36.67443	41.39017
N	72.80947	-35.21257	41.31213
C	73.03790	-34.41809	42.35664
N	73.05547	-34.92047	43.59499
N	73.22897	-33.10011	42.16346
C*	79.04600	-41.17200	35.58000
O	78.28520	-41.93565	34.99998
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17424	-43.77572	37.78037
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69922	-39.60962	40.66426
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.61981	-39.32228	37.26737
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46683	-36.19125	41.25398
Fe	76.99603	-37.96505	39.85797
Fe	78.45105	-36.80290	37.62856
Fe	76.90570	-35.32123	39.49329
Fe	79.34439	-36.54282	40.37030
S	79.01331	-34.83753	38.74569
S	77.37305	-36.37253	41.56523



S	79.09101	-38.50952	39.07609
S	76.16639	-36.88127	37.92931
H	77.53375	-32.13970	45.86718
H	77.75862	-32.11807	44.13684
H	77.02690	-34.55627	45.89234
H	76.76169	-34.59747	44.14650
H	79.54012	-34.02696	45.38692
H	79.15461	-34.27476	43.67541
H	78.89012	-36.40540	45.87052
H	78.31754	-36.60132	44.21667
H	80.47419	-36.67243	43.35393
H	82.39109	-36.06778	46.86671
H	80.67487	-36.24526	46.90393
H	82.64746	-36.48675	43.35010
H	75.57736	-31.06838	44.64038
H	73.44578	-32.53475	42.97842
H	82.02498	-33.51707	42.63810
H	81.57165	-32.53200	44.05941
H	82.37457	-31.76742	42.66226
H	79.95811	-30.24235	42.83060
H	77.63158	-30.48951	41.82731
H	77.45907	-32.95763	41.06183
H	79.61796	-34.20977	41.42444
H	75.25652	-31.73735	37.31288
H	76.44504	-30.50561	37.76876
H	76.57981	-31.56674	39.74936
H	77.58265	-32.75287	38.92864
H	76.78840	-33.98611	36.70290
H	77.68907	-33.29026	34.12566
H	79.14574	-33.56981	35.08967
H	78.04773	-35.51125	33.65155
H	76.89827	-35.69905	34.98616
H	71.74781	-37.77840	38.20986
H	71.24793	-36.24622	38.95746
H	70.76690	-37.79218	39.69940
H	73.71351	-36.83952	39.45191
H	73.18699	-38.34315	40.16062
H	73.70722	-36.98772	41.95987
H	71.91839	-37.02645	41.93255
H	72.72757	-34.77634	40.39825
H	72.81726	-35.88759	43.77397
H	73.48236	-34.38028	44.34203
H	73.63948	-32.81692	41.27226
H	79.43608	-40.23683	35.11128
H	80.20179	-40.67621	37.15182
H	79.45499	-43.43753	37.02147
H	79.84092	-41.43936	39.36234
H	81.14758	-42.33616	38.53579
H	79.95429	-43.21291	39.52704
H	77.52714	-40.73091	38.46507
H	75.32101	-42.31818	39.43034
H	75.06566	-41.92110	37.71768
H	74.02342	-40.16808	39.02969
H	75.42691	-39.47044	38.22420
H	83.56464	-36.47549	44.85219
H	83.27753	-41.35866	37.04196
H	83.98788	-40.11500	36.00640
H	84.70398	-40.43416	37.61303
H	84.36258	-38.58315	38.61008
H	81.85122	-37.06411	38.31659
H	83.13077	-37.90171	40.99155
H	81.56456	-38.45472	40.37318
H	83.41615	-36.44846	38.92749

**Table S6.9 Menaquinone stacked, SQ N2[ox]**

209

# E=-12300.35454245 Hartree			
C	71.18378	-25.19159	32.74826
C	72.22834	-24.60635	31.91971
C	73.47772	-24.21878	32.59742
C	73.60405	-24.32857	34.00801
C	72.52349	-24.90037	34.81402
C	71.33225	-25.33626	34.13050
C	69.90656	-25.58204	32.05436
C*	70.21510	-25.92740	34.97980
C	70.19778	-27.43668	34.96716
C	69.18529	-28.24187	34.60790
C	67.81564	-27.84598	34.12992
O	72.09044	-24.41751	30.68506
O	72.66575	-24.98535	36.08320
C*	67.24000	-22.83800	33.62700
C	69.73802	-22.28671	34.04558
C	68.48421	-22.01072	33.53845
N	70.54570	-21.23716	33.66807
N	68.53841	-20.80417	32.86153
C	69.78892	-20.37618	32.95975
C*	76.92100	-28.86700	39.93100
C	75.66091	-28.41741	39.24024
C	75.67682	-27.34061	38.34054
C	74.51132	-26.87266	37.73829
C	73.26944	-27.48062	38.02226
O	72.11548	-27.04186	37.50657
C	74.42598	-29.03719	39.49209
C	73.24782	-28.58587	38.89604
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.50416	-20.30253	31.73899
O	73.26896	-20.96252	32.98576
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.09240	-18.50832	30.48254
O	67.26816	-19.39743	31.00644
O	69.22690	-18.29229	30.87916
H	69.62265	-26.62119	32.28151
H	70.01960	-25.46465	30.96899
H	69.06973	-24.93772	32.37965
H	70.35882	-25.58744	36.01808
H	69.24487	-25.52769	34.64906
H	71.13055	-27.89753	35.30870
H	69.36088	-29.32442	34.66808
H	67.68255	-26.75657	34.06319
H	67.03341	-28.24058	34.80333
H	67.60889	-28.27028	33.13094
H	66.40930	-22.27412	34.08425
H	67.41546	-23.74001	34.23235
H	66.90536	-23.15902	32.62569
H	70.11642	-23.13413	34.60706
H	71.57215	-21.16787	33.70648
H	67.70954	-19.94201	31.76581
H	70.15787	-19.46211	32.50062
H	77.59472	-28.01937	40.13623
H	77.50595	-29.60206	39.35111
H	76.66197	-29.31629	40.90290
H	76.62312	-26.84133	38.11655
H	74.52991	-26.01869	37.05963
H	72.26978	-26.21813	36.93477
H	74.37900	-29.88507	40.18538
H	72.28698	-29.06144	39.10853
H	78.02573	-23.98330	40.32128
H	76.70717	-22.94384	40.92387
H	77.86945	-22.31045	39.73087
H	75.82709	-24.56454	39.24191
H	75.90219	-21.69091	38.12855
H	74.81032	-22.25262	39.42141
H	74.65639	-22.92041	37.78135

H	77.68056	-23.21136	37.19899
H	76.50365	-24.50434	36.87287
H	77.93878	-24.84014	37.86360
H	73.39701	-19.22322	31.93840
H	74.55417	-20.47193	31.43330
H	73.55314	-21.88543	32.88482
H	71.52332	-20.42258	30.82239
H	72.56544	-21.83138	30.49619
H	72.87041	-20.27544	29.66817
H	68.18470	-17.00195	28.94808
H	66.53396	-17.30570	29.61005
H	67.26257	-18.48316	28.50347
H	74.85850	-23.94155	35.70896
C	74.79536	-23.88162	34.62324
C	75.84764	-23.37891	33.87094
H	76.76074	-23.03814	34.36701
C	75.73755	-23.30840	32.46480
H	76.56831	-22.92177	31.86825
C	74.56410	-23.71954	31.84279
H	74.44321	-23.66138	30.75925
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.04655	-36.07560	44.82168
N	80.34930	-36.52732	44.34377
C	81.50090	-36.43074	45.01490
N	81.51182	-36.22584	46.34152
N	82.65124	-36.53092	44.34159
C*	75.72200	-32.17300	44.73700
O	74.76938	-32.91863	44.68232
C*	81.64500	-32.53700	42.95900
N	79.57792	-31.14828	42.45162
C	80.31533	-32.31718	42.34155
C	78.36177	-31.32301	41.92153
N	78.29767	-32.57589	41.47295
C	79.49685	-33.20543	41.69720
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.40354	-33.60230	39.57680
C*	77.25800	-32.00400	36.55700
O	77.93412	-31.14865	35.98254
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.12684	-36.54759	35.49178
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.81383	-36.66478	41.38592
N	72.81271	-35.20323	41.30156
C	73.04329	-34.40711	42.34479
N	73.05405	-34.90798	43.58465
N	73.24229	-33.09148	42.15139
C*	79.04600	-41.17200	35.58000
O	78.29148	-41.94038	34.99773
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17578	-43.77724	37.78408
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69384	-39.61236	40.66680
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62018	-39.32276	37.26675
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.47048	-36.18493	41.24474
Fe	76.99411	-37.97127	39.85520
Fe	78.44734	-36.81344	37.62220
Fe	76.90290	-35.32835	39.48000
Fe	79.34023	-36.55045	40.37345
S	79.01183	-34.85103	38.73683
S	77.36598	-36.37388	41.55907

S	79.08950	-38.51777	39.07374
S	76.16418	-36.89174	37.92313
H	77.53204	-32.14034	45.86825
H	77.75985	-32.11758	44.13908
H	77.02602	-34.55730	45.89158
H	76.76255	-34.59648	44.14517
H	79.54053	-34.03636	45.39359
H	79.15818	-34.26740	43.67807
H	78.88091	-36.41309	45.85785
H	78.29630	-36.59176	44.20634
H	80.44960	-36.66306	43.32736
H	82.38889	-36.19309	46.84754
H	80.66997	-36.35230	46.88972
H	82.61826	-36.50455	43.31776
H	75.57717	-31.06901	44.63550
H	73.45281	-32.52271	42.96530
H	82.04250	-33.50791	42.63160
H	81.56356	-32.54329	44.05884
H	82.36492	-31.75338	42.67533
H	79.90394	-30.27577	42.86174
H	77.58481	-30.56941	41.85408
H	77.47331	-33.02309	41.04953
H	79.67467	-34.22279	41.37953
H	75.25668	-31.73843	37.31241
H	76.43862	-30.50568	37.77168
H	76.58256	-31.56282	39.74646
H	77.58298	-32.75163	38.92710
H	76.76760	-33.98039	36.68597
H	77.68944	-33.29207	34.12436
H	79.14540	-33.56876	35.08997
H	78.04740	-35.51117	33.65151
H	76.89836	-35.69930	34.98605
H	71.74410	-37.78818	38.21439
H	71.25442	-36.24627	38.94808
H	70.76400	-37.78227	39.70463
H	73.71546	-36.84600	39.44967
H	73.18281	-38.34326	40.16856
H	73.70292	-36.97860	41.96006
H	71.91415	-37.01096	41.92743
H	72.73922	-34.76946	40.38562
H	72.81904	-35.87610	43.76142
H	73.48914	-34.37152	44.32985
H	73.64512	-32.80581	41.25751
H	79.43012	-40.23341	35.11343
H	80.19695	-40.67249	37.15470
H	79.45499	-43.43738	37.02120
H	79.84035	-41.43965	39.36249
H	81.14750	-42.33530	38.53563
H	79.95461	-43.21328	39.52673
H	77.52609	-40.72987	38.46098
H	75.32138	-42.31828	39.43038
H	75.06591	-41.92143	37.71758
H	74.02333	-40.16710	39.02545
H	75.42936	-39.47056	38.22509
H	83.54527	-36.57195	44.81530
H	83.27303	-41.35614	37.02947
H	83.99901	-40.10708	36.01082
H	84.69862	-40.44294	37.62112
H	84.36283	-38.58249	38.60908
H	81.85094	-37.06392	38.31708
H	83.13015	-37.90259	40.99220
H	81.56251	-38.45315	40.37339
H	83.41606	-36.44842	38.92762

Table S6.10 Menaquinone H-bonded, Q N2[red]

209

# E=-12300.34920984 Hartree

C	71.88279	-25.40094	35.51943
C	71.47714	-25.03232	36.91019
C	71.67233	-23.63491	37.37539
C	72.24438	-22.67970	36.51499
C	72.62637	-23.06134	35.13065
C	72.40641	-24.46360	34.67483
C	71.61748	-26.81144	35.07812
C*	72.67300	-24.74800	33.21300
C	71.38624	-24.59532	32.42500
C	70.78482	-25.52154	31.66316
C	71.23497	-26.92611	31.38485
O	70.98625	-25.86516	37.66946
O	73.08315	-22.21083	34.36995
C*	67.24000	-22.83800	33.62700
C	69.50430	-21.95758	34.52044
C	68.45306	-21.96329	33.62768
N	70.36652	-20.97134	34.08363
N	68.68275	-20.99463	32.66823
C	69.83813	-20.42294	32.96734
C*	76.92100	-28.86700	39.93100
C	75.47648	-28.75300	39.51729
C	75.04313	-27.71103	38.68562
C	73.70729	-27.59523	38.29432
C	72.75586	-28.53261	38.73011
O	71.44673	-28.47043	38.38721
C	74.51431	-29.68744	39.93989
C	73.17827	-29.59061	39.55428
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.60256	-20.36437	31.66891
O	74.42977	-21.45900	32.03037
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.19043	-18.68866	30.28401
O	67.39605	-19.63933	30.74935
O	69.35974	-18.55232	30.60776
H	70.79037	-26.82644	34.34790
H	71.34750	-27.45911	35.91903
H	72.49640	-27.24145	34.57506
H	73.40115	-24.01760	32.82896
H	73.10814	-25.74804	33.08843
H	70.91113	-23.61139	32.51538
H	69.85398	-25.22091	31.16499
H	72.16292	-27.19742	31.90864
H	71.40391	-27.07110	30.30326
H	70.45472	-27.65135	31.67573
H	66.31732	-22.24125	33.72153
H	67.27453	-23.55530	34.46008
H	67.16620	-23.40608	32.68470
H	69.69323	-22.54895	35.41101
H	71.27027	-20.73870	34.48100
H	67.87298	-20.21608	31.44647
H	70.29434	-19.61824	32.39438
H	77.50648	-28.00626	39.57391
H	77.40941	-29.76887	39.53193
H	77.01823	-28.87876	41.03118
H	75.76507	-26.97157	38.32639
H	73.40637	-26.77772	37.64007
H	71.22424	-27.57916	38.04685
H	74.81232	-30.51882	40.58596
H	72.44043	-30.32369	39.88886
H	78.02405	-23.98338	40.32331
H	76.70766	-22.94040	40.92306
H	77.87009	-22.31280	39.72665
H	75.82341	-24.56352	39.24437
H	75.90503	-21.67408	38.17146
H	74.77190	-22.28352	39.40551
H	74.69359	-22.90145	37.74251
H	77.73781	-23.22733	37.24053

H	76.48905	-24.43284	36.84537
H	77.88640	-24.89421	37.84786
H	73.10231	-19.94135	32.56355
H	74.25561	-19.56492	31.27291
H	74.04092	-21.86347	32.82185
H	71.89341	-21.52699	31.00483
H	73.04851	-21.11752	29.71072
H	71.93054	-19.86989	30.35113
H	68.19565	-17.03280	28.90814
H	66.66342	-17.25244	29.82894
H	67.04116	-18.35576	28.49388
H	70.86449	-24.02660	39.33084
C	71.30235	-23.27100	38.67624
C	71.49756	-21.95788	39.11499
H	71.20548	-21.67441	40.12893
C	72.07213	-21.00873	38.26075
H	72.23455	-19.98585	38.60834
C	72.45016	-21.36959	36.96483
H	72.92396	-20.64631	36.29839
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.03701	-36.07865	44.79521
N	80.34012	-36.52530	44.31573
C	81.49025	-36.39650	44.98108
N	81.49652	-36.16311	46.30628
N	82.64081	-36.48898	44.30843
C*	75.72200	-32.17300	44.73700
O	74.77332	-32.92020	44.65061
C*	81.64500	-32.53700	42.95900
N	79.54477	-31.20304	42.39046
C	80.31186	-32.35789	42.33167
C	78.33297	-31.43457	41.86532
N	78.30457	-32.70603	41.47088
C	79.51720	-33.29152	41.72442
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39403	-33.59416	39.55068
C*	77.25800	-32.00400	36.55700
O	77.90179	-31.13798	35.95499
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.19460	-36.53250	35.39453
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.83420	-36.61545	41.36304
N	72.85791	-35.15573	41.22426
C	73.02707	-34.32276	42.24959
N	72.87373	-34.75745	43.50647
N	73.31914	-33.02861	42.01509
C*	79.04600	-41.17200	35.58000
O	78.32161	-41.96006	34.98288
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17259	-43.77573	37.76727
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.63268	-39.62826	40.69188
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62605	-39.31826	37.25228
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.47074	-36.20967	41.26789
Fe	76.97817	-37.95663	39.90644
Fe	78.45007	-36.92938	37.52495
Fe	76.90214	-35.37965	39.46789
Fe	79.32483	-36.50481	40.38559
S	79.00577	-34.85137	38.75673
S	77.29306	-36.32756	41.60865
S	79.06605	-38.57319	39.22844

S	76.10959	-36.94324	37.95005
H	77.53592	-32.13716	45.86523
H	77.75602	-32.11921	44.13447
H	77.02395	-34.55764	45.89098
H	76.76714	-34.59517	44.14118
H	79.54099	-34.04874	45.40272
H	79.15956	-34.25703	43.68356
H	78.86252	-36.43621	45.82411
H	78.29010	-36.57365	44.15846
H	80.44009	-36.66192	43.29539
H	82.37257	-36.13660	46.81385
H	80.65637	-36.30829	46.85250
H	82.59378	-36.46741	43.27944
H	75.57545	-31.06586	44.66285
H	73.50632	-32.44860	42.82661
H	82.05137	-33.51494	42.66347
H	81.56423	-32.50784	44.05873
H	82.35716	-31.75626	42.64836
H	79.84710	-30.30644	42.76312
H	77.53522	-30.70729	41.76791
H	77.50030	-33.20178	41.05748
H	79.72163	-34.31980	41.46067
H	75.25764	-31.74097	37.31197
H	76.44260	-30.50504	37.76563
H	76.61003	-31.57244	39.75242
H	77.57206	-32.78084	38.91688
H	76.86761	-34.00389	36.76048
H	77.69091	-33.27638	34.13297
H	79.14753	-33.57454	35.09120
H	77.94833	-35.49407	33.64168
H	76.92188	-35.70403	35.06595
H	71.73767	-37.81271	38.22677
H	71.27091	-36.24612	38.92509
H	70.75462	-37.75733	39.71428
H	73.72685	-36.89000	39.43298
H	73.16590	-38.34213	40.20464
H	73.71987	-36.92697	41.94415
H	71.92721	-36.91862	41.91770
H	72.96355	-34.76756	40.29000
H	72.62582	-35.72056	43.69401
H	73.28756	-34.21783	44.26092
H	73.88596	-32.85034	41.17286
H	79.40163	-40.21603	35.12681
H	80.14993	-40.63916	37.18238
H	79.45404	-43.43566	37.01818
H	79.84333	-41.43550	39.35676
H	81.14770	-42.33938	38.53530
H	79.95085	-43.21104	39.52924
H	77.53553	-40.73791	38.51759
H	75.31848	-42.32046	39.42832
H	75.07262	-41.92421	37.71428
H	74.02290	-40.15838	38.97735
H	75.46598	-39.46382	38.24693
H	83.53600	-36.48307	44.78091
H	83.25595	-41.34473	36.97900
H	84.04319	-40.07595	36.03030
H	84.67652	-40.48065	37.65154
H	84.35709	-38.59564	38.62791
H	81.84784	-37.06686	38.31998
H	83.13239	-37.92319	40.98096
H	81.54950	-38.44210	40.35813
H	83.41674	-36.44814	38.92376

**Table S6.11 Menaquinone H-bonded, Q N2[ox]**

209

# E=-12300.21290903 Hartree

C	71.88086	-25.38726	35.52222
C	71.47429	-25.01090	36.91003
C	71.67649	-23.61367	37.37090
C	72.25168	-22.66356	36.50675
C	72.63174	-23.05153	35.12374
C	72.40780	-24.45568	34.67345
C	71.60964	-26.79811	35.08481
C*	72.67300	-24.74800	33.21300
C	71.38549	-24.59902	32.42530
C	70.78598	-25.52736	31.66449
C	71.23901	-26.93117	31.38745
O	70.97526	-25.83871	37.67090
O	73.09032	-22.20613	34.35925
C*	67.24000	-22.83800	33.62700
C	69.50505	-21.95804	34.52037
C	68.45249	-21.96261	33.62908
N	70.36470	-20.96837	34.08586
N	68.67906	-20.99005	32.67296
C	69.83339	-20.41699	32.97228
C*	76.92100	-28.86700	39.93100
C	75.48001	-28.74081	39.50615
C	75.05452	-27.68475	38.68822
C	73.72089	-27.55826	38.29169
C	72.76341	-28.49831	38.70924
O	71.45791	-28.43247	38.36083
C	74.51180	-29.67690	39.91224
C	73.17828	-29.56853	39.52212
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.61004	-20.36689	31.66200
O	74.43602	-21.46453	32.01910
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.18760	-18.68649	30.28728
O	67.39095	-19.63460	30.75443
O	69.35678	-18.55169	30.61242
H	70.77776	-26.81213	34.36007
H	71.34331	-27.44452	35.92765
H	72.48402	-27.23036	34.57599
H	73.40081	-24.01968	32.82425
H	73.10774	-25.74886	33.09354
H	70.90881	-23.61576	32.51392
H	69.85490	-25.22903	31.16557
H	72.16747	-27.20012	31.91177
H	71.40872	-27.07632	30.30599
H	70.45988	-27.65771	31.67815
H	66.31791	-22.24330	33.73878
H	67.28238	-23.56723	34.44935
H	67.15763	-23.39198	32.67713
H	69.69551	-22.55133	35.40931
H	71.26679	-20.73180	34.48433
H	67.86707	-20.21057	31.45162
H	70.28702	-19.60949	32.40110
H	77.51987	-28.01638	39.57226
H	77.40467	-29.77742	39.54560
H	77.00347	-28.86326	41.03205
H	75.78044	-26.94198	38.34464
H	73.42649	-26.72964	37.64830
H	71.23053	-27.53554	38.03433
H	74.80254	-30.51476	40.55413
H	72.43177	-30.29848	39.84429
H	78.02413	-23.98336	40.32357
H	76.70762	-22.93998	40.92285
H	77.87019	-22.31301	39.72662
H	75.82308	-24.56323	39.24490
H	75.90503	-21.67416	38.17163
H	74.77215	-22.28354	39.40560
H	74.69351	-22.90126	37.74248
H	77.73714	-23.22718	37.24022



H	76.48918	-24.43317	36.84533
H	77.88745	-24.89347	37.84796
H	73.11666	-19.94230	32.55964
H	74.26340	-19.56992	31.26183
H	74.04958	-21.86633	32.81282
H	71.89173	-21.52306	31.01007
H	73.04184	-21.12155	29.70886
H	71.93301	-19.86770	30.35251
H	68.19652	-17.03364	28.90818
H	66.66195	-17.25142	29.82552
H	67.04326	-18.35757	28.49402
H	70.86829	-23.99484	39.32866
C	71.30935	-23.24371	38.67110
C	71.51057	-21.93010	39.10536
H	71.22072	-21.64184	40.11858
C	72.08730	-20.98586	38.24697
H	72.25320	-19.96224	38.59057
C	72.46271	-21.35264	36.95189
H	72.93796	-20.63295	36.28254
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05808	-36.07301	44.83246
N	80.36938	-36.51321	44.36594
C	81.51663	-36.37276	45.03712
N	81.51721	-36.12024	46.35554
N	82.67210	-36.47497	44.37283
C*	75.72200	-32.17300	44.73700
O	74.76915	-32.91768	44.67628
C*	81.64500	-32.53700	42.95900
N	79.60773	-31.11503	42.43238
C	80.31349	-32.30501	42.34950
C	78.38896	-31.26609	41.90153
N	78.29132	-32.52716	41.48069
C	79.47095	-33.18566	41.72435
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.39453	-33.58966	39.58351
C*	77.25800	-32.00400	36.55700
O	77.92190	-31.14445	35.97348
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.12676	-36.54362	35.49665
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.81542	-36.66914	41.38771
N	72.81097	-35.20687	41.30506
C	73.03842	-34.41000	42.34770
N	73.05492	-34.91016	43.58660
N	73.22874	-33.09105	42.15188
C*	79.04600	-41.17200	35.58000
O	78.28513	-41.93562	35.00006
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17423	-43.77572	37.78044
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69839	-39.60924	40.66444
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.61971	-39.32229	37.26762
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46635	-36.19154	41.25409
Fe	76.99359	-37.96308	39.85919
Fe	78.44814	-36.80112	37.63034
Fe	76.90266	-35.31890	39.49601
Fe	79.34294	-36.54254	40.37219
S	79.01139	-34.83709	38.74802
S	77.37099	-36.37132	41.56687
S	79.08830	-38.50825	39.07707

S	76.16326	-36.87800	37.93154
H	77.53414	-32.13936	45.86684
H	77.75829	-32.11835	44.13630
H	77.02690	-34.55634	45.89231
H	76.76169	-34.59739	44.14645
H	79.54000	-34.02734	45.38734
H	79.15479	-34.27446	43.67576
H	78.88962	-36.40592	45.86987
H	78.31732	-36.60105	44.21587
H	80.47402	-36.67289	43.35358
H	82.39080	-36.06689	46.86612
H	80.67460	-36.24449	46.90329
H	82.64721	-36.48660	43.34959
H	75.57753	-31.06826	44.64022
H	73.44430	-32.52523	42.96693
H	82.02541	-33.51700	42.63818
H	81.57273	-32.53179	44.05954
H	82.37366	-31.76707	42.66126
H	79.95894	-30.24446	42.82550
H	77.63381	-30.49301	41.81687
H	77.45966	-32.96079	41.05905
H	79.61638	-34.21503	41.42945
H	75.25620	-31.73500	37.31349
H	76.44632	-30.50651	37.77102
H	76.60130	-31.56531	39.74581
H	77.57776	-32.76367	38.92019
H	76.78927	-33.98624	36.70366
H	77.68906	-33.29030	34.12567
H	79.14573	-33.56978	35.08965
H	78.04896	-35.51154	33.65174
H	76.89791	-35.69872	34.98516
H	71.74751	-37.77915	38.21021
H	71.24850	-36.24621	38.95676
H	70.76666	-37.79139	39.69979
H	73.71381	-36.84163	39.45067
H	73.18610	-38.34292	40.16376
H	73.70695	-36.98095	41.95895
H	71.91799	-37.01813	41.93093
H	72.72813	-34.77328	40.38995
H	72.81736	-35.87738	43.76620
H	73.48143	-34.36955	44.33365
H	73.65145	-32.81260	41.26444
H	79.43612	-40.23688	35.11123
H	80.20192	-40.67630	37.15176
H	79.45500	-43.43754	37.02149
H	79.84090	-41.43937	39.36236
H	81.14757	-42.33612	38.53578
H	79.95431	-43.21292	39.52703
H	77.52709	-40.73088	38.46490
H	75.32099	-42.31819	39.43032
H	75.06560	-41.92100	37.71768
H	74.02341	-40.16809	39.02943
H	75.42700	-39.47048	38.22418
H	83.56447	-36.47427	44.85162
H	83.27762	-41.35871	37.04217
H	83.98770	-40.11514	36.00632
H	84.70406	-40.43397	37.61291
H	84.36264	-38.58301	38.60990
H	81.85124	-37.06408	38.31658
H	83.13074	-37.90155	40.99165
H	81.56464	-38.45480	40.37317
H	83.41617	-36.44847	38.92751

**Table S6.12 Menaquinone H-bonded, SQ N2[ox]**

209

# E=-12300.36377795 Hartree

C	71.90200	-25.40371	35.54548
C	71.52424	-25.07549	36.90467
C	71.73934	-23.69957	37.36580
C	72.29077	-22.72680	36.49466
C	72.65637	-23.08147	35.12074
C	72.43040	-24.43779	34.68229
C	71.65125	-26.81104	35.06521
C*	72.67300	-24.74800	33.21300
C	71.40024	-24.64393	32.40343
C	70.82246	-25.58527	31.64112
C	71.29394	-26.99061	31.39336
O	71.01396	-25.92334	37.70302
O	73.08189	-22.16477	34.34048
C*	67.24000	-22.83800	33.62700
C	69.63873	-22.18810	34.29871
C	68.48337	-22.01202	33.57124
N	70.51925	-21.22025	33.86566
N	68.66271	-20.94409	32.70884
C	69.89738	-20.50187	32.90778
C*	76.92100	-28.86700	39.93100
C	75.48422	-28.73892	39.49480
C	75.07113	-27.67923	38.67249
C	73.74207	-27.53252	38.27407
C	72.76668	-28.46244	38.68829
O	71.47398	-28.36591	38.34412
C	74.50469	-29.66318	39.89868
C	73.17361	-29.54026	39.50160
C*	77.29700	-23.20700	40.03000
C*	76.39200	-23.68200	38.89000
C*	75.38300	-22.57600	38.53600
C*	77.16700	-24.08300	37.64200
C	73.60109	-20.40416	31.68664
O	74.36906	-21.52702	32.07088
C*	72.55900	-20.73500	30.62100
C*	67.48800	-17.76800	29.31100
C	68.17758	-18.63668	30.34287
O	67.37297	-19.54540	30.86338
O	69.35022	-18.49251	30.65211
H	70.88514	-26.82505	34.27202
H	71.31391	-27.45568	35.88481
H	72.56124	-27.25782	34.63208
H	73.37562	-24.00042	32.81230
H	73.14097	-25.73538	33.09418
H	70.90654	-23.66860	32.46920
H	69.89356	-25.30664	31.12562
H	72.21261	-27.23785	31.94480
H	71.48971	-27.15661	30.31857
H	70.51879	-27.72230	31.68400
H	66.35290	-22.22574	33.86337
H	67.33197	-23.62204	34.39297
H	67.04631	-23.32812	32.65737
H	69.90320	-22.92183	35.05351
H	71.52266	-21.20650	34.09593
H	67.85051	-20.11945	31.58000
H	70.34726	-19.67644	32.36101
H	77.52682	-28.02934	39.55325
H	77.40570	-29.78871	39.57221
H	77.00533	-28.83830	41.03304
H	75.80682	-26.94387	38.33238
H	73.45297	-26.69531	37.63924
H	71.27163	-27.43884	38.00050
H	74.78409	-30.50120	40.54698
H	72.41761	-30.26116	39.82375
H	78.02649	-23.98157	40.32471
H	76.70690	-22.94041	40.92271
H	77.86831	-22.31131	39.72693
H	75.82321	-24.56357	39.24364
H	75.90679	-21.67468	38.17170
H	74.77227	-22.28308	39.40505
H	74.68929	-22.89897	37.74656
H	77.73770	-23.22679	37.24102

H	76.48663	-24.42932	36.84642
H	77.88685	-24.89516	37.84627
H	73.10146	-19.95089	32.56710
H	74.28866	-19.62966	31.29431
H	73.96045	-21.88956	32.88683
H	71.86328	-21.50425	30.99552
H	73.04881	-21.13552	29.71806
H	71.96510	-19.84856	30.34143
H	68.19801	-17.04535	28.88956
H	66.64418	-17.23850	29.78162
H	67.06937	-18.39994	28.51173
H	70.98096	-24.10042	39.33881
C	71.39543	-23.33059	38.68492
C	71.57859	-22.02663	39.12628
H	71.30690	-21.75083	40.14928
C	72.11548	-21.05535	38.25486
H	72.26127	-20.02929	38.60384
C	72.46908	-21.40474	36.95934
H	72.90196	-20.67314	36.27484
C*	77.18100	-32.61600	44.93300
C*	77.38500	-34.14300	44.93500
C*	78.86799	-34.55900	44.69100
C	79.05679	-36.07308	44.83038
N	80.36730	-36.51366	44.36169
C	81.51518	-36.37255	45.03105
N	81.51763	-36.12127	46.34975
N	82.66988	-36.47536	44.36516
C*	75.72200	-32.17300	44.73700
O	74.77074	-32.91854	44.66881
C*	81.64500	-32.53700	42.95900
N	79.57653	-31.14321	42.44758
C	80.31143	-32.31515	42.34509
C	78.35836	-31.31749	41.92027
N	78.29083	-32.57368	41.48046
C	79.48867	-33.20498	41.70775
C*	76.29600	-31.58300	37.64700
C*	76.57100	-32.33800	38.96800
S	75.40419	-33.60009	39.57809
C*	77.25800	-32.00400	36.55700
O	77.93040	-31.14792	35.97897
N*	77.36100	-33.31100	36.20100
C*	78.07701	-33.82500	35.01000
C*	77.92100	-35.37700	34.73500
S	79.12920	-36.54742	35.48857
C*	71.58700	-37.27400	39.17500
C*	72.87900	-37.29900	40.00900
C	72.82060	-36.63528	41.37294
N	72.80817	-35.17510	41.25952
C	73.01813	-34.35683	42.29004
N	73.02028	-34.83408	43.53838
N	73.20631	-33.04174	42.07312
C*	79.04600	-41.17200	35.58000
O	78.28891	-41.93858	34.99869
N*	79.48900	-41.34100	36.83400
C*	79.20900	-42.52700	37.59000
C*	80.08700	-42.37100	38.83000
C*	77.70900	-42.67700	37.91600
O	77.17461	-43.77620	37.78019
N*	77.03399	-41.62000	38.40700
C*	75.58700	-41.60000	38.63700
C*	75.12400	-40.17100	39.01400
S	75.69745	-39.61155	40.66540
C*	83.75900	-40.36900	37.05500
C*	82.81000	-39.35800	37.59000
O	81.62024	-39.32286	37.26658
N*	83.37500	-38.47700	38.40900
C*	82.72300	-37.30300	38.94400
C*	82.25300	-37.60100	40.39600
S	81.46634	-36.19286	41.25341
Fe	76.99439	-37.96832	39.85328
Fe	78.45193	-36.81104	37.62168
Fe	76.90549	-35.32550	39.47955
Fe	79.34331	-36.54912	40.36489
S	79.01616	-34.84798	38.73575
S	77.37236	-36.37227	41.55675
S	79.09003	-38.51741	39.07315

S	76.16693	-36.88805	37.92135
H	77.53259	-32.14043	45.86799
H	77.75951	-32.11742	44.13880
H	77.02636	-34.55655	45.89207
H	76.76186	-34.59702	44.14611
H	79.54041	-34.02813	45.38756
H	79.15491	-34.27378	43.67557
H	78.88938	-36.40763	45.86752
H	78.31503	-36.59957	44.21359
H	80.47079	-36.67095	43.34866
H	82.39148	-36.06343	46.85909
H	80.67433	-36.23835	46.89780
H	82.64241	-36.48072	43.34155
H	75.57681	-31.06771	44.64811
H	73.39102	-32.45101	42.87730
H	82.03368	-33.51387	42.63889
H	81.56934	-32.53115	44.05919
H	82.36799	-31.76096	42.66266
H	79.90562	-30.26914	42.85196
H	77.58297	-30.56198	41.84874
H	77.46485	-33.02195	41.06064
H	79.66237	-34.22529	41.39715
H	75.25555	-31.73307	37.31461
H	76.44458	-30.50659	37.77374
H	76.59058	-31.56760	39.74800
H	77.58110	-32.75605	38.92310
H	76.77241	-33.98160	36.69012
H	77.68946	-33.29150	34.12470
H	79.14548	-33.56895	35.08993
H	78.04425	-35.51094	33.65112
H	76.89912	-35.69949	34.98896
H	71.74262	-37.79229	38.21636
H	71.25737	-36.24627	38.94386
H	70.76228	-37.77756	39.70647
H	73.71933	-36.86456	39.44073
H	73.17244	-38.34296	40.18920
H	73.71566	-36.93048	41.94755
H	71.92678	-36.97589	41.92757
H	72.72447	-34.75948	40.33613
H	72.78715	-35.79974	43.73054
H	73.45216	-34.28437	44.27611
H	73.63454	-32.77317	41.18520
H	79.43243	-40.23478	35.11257
H	80.19817	-40.67342	37.15396
H	79.45486	-43.43743	37.02123
H	79.84096	-41.43925	39.36208
H	81.14758	-42.33605	38.53578
H	79.95410	-43.21285	39.52715
H	77.52744	-40.73106	38.46737
H	75.32108	-42.31819	39.43042
H	75.06620	-41.92154	37.71749
H	74.02336	-40.16721	39.02797
H	75.42790	-39.47074	38.22433
H	83.56303	-36.46564	44.84219
H	83.27667	-41.35822	37.04013
H	83.98942	-40.11376	36.00703
H	84.70330	-40.43561	37.61412
H	84.36263	-38.58292	38.60977
H	81.85113	-37.06404	38.31673
H	83.13107	-37.90218	40.99109
H	81.56513	-38.45526	40.37221
H	83.41602	-36.44835	38.92722

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