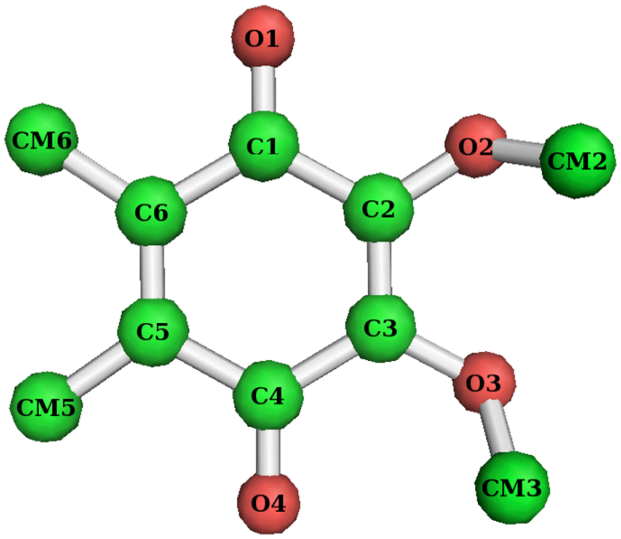


| Atom | UQ | $SQ^-$ |
|---|---|---|
| O1 | -0.41 | -0.57 |
| C1 | 0.40 | 0.32 |
| C2 | 0.08 | 0.09 |
| O2 | -0.32 | -0.36 |
| CM2 | 0.25 | 0.17 |
| C3 | 0.09 | 0.08 |
| CM3 | 0.24 | 0.16 |
| C4 | 0.42 | 0.32 |
| O4 | -0.41 | -0.57 |
| C5 | -0.12 | -0.19 |
| CM5 | 0.11 | 0.06 |
| O3 | -0.32 | -0.37 |
| C6 | -0.14 | -0.20 |
| CM6 | 0.13 | 0.06 |

Figure S1: Partial atomic charges for UQ and $SQ^-$ derived from DFT in the Gaussian 98 program at the UB3LYP/6-31G level of theory. These charge sets were used for MCCE, not SMD, calculations.

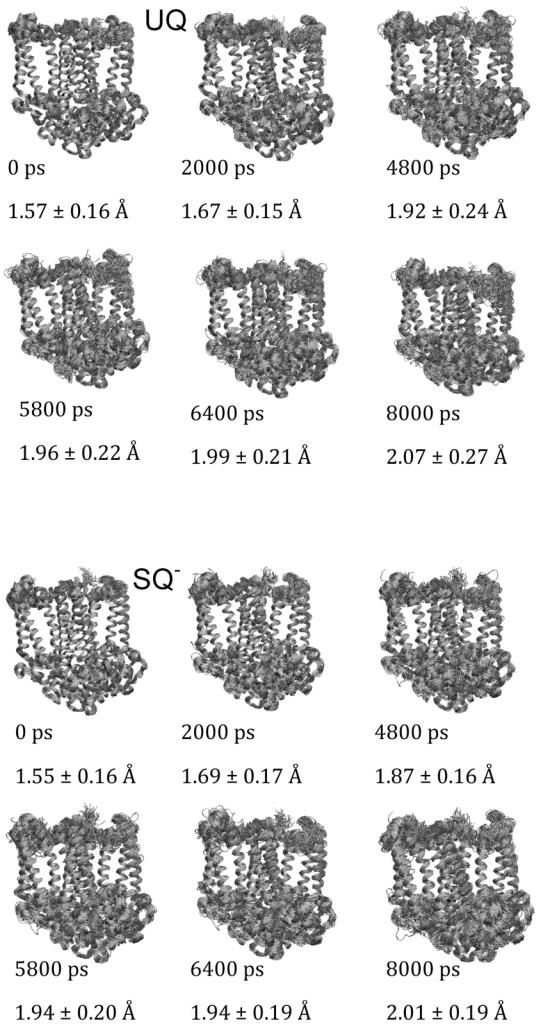


Figure S2: Superimposed structures of reaction center with bound ubiquinone (UQ) or semiquinone ($SQ^-$), obtained during 45 steered MD simulations and shown at selected times, as indicated in the figure. Average RMSD values of the 45 structure, relative to the crystal structure, are shown in the graphs.

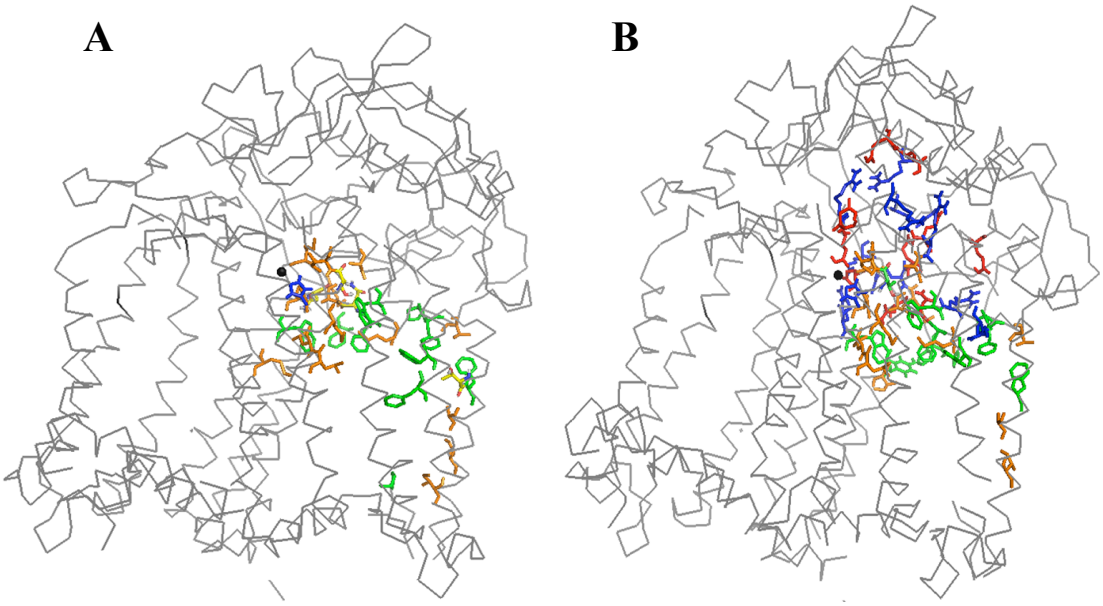


Figure S3: Residues involved in pair wise interactions (at least 1 kcal/mol) with quinone head group along UQ (A) and $SQ^-$ (B) pathways highlighted on RC backbone. Fe2+ is shown as a black sphere and the HIS M219 ligand, shown in blue sticks. Residues are categorized as blue bases (LYS, ARG, HIS); red acids (ASP, GLU); orange hydrophobic (ILE, LEU, VAL, ALA); green aromatic (PHE, TRP, TYR). There are more acidic and basic amino acids interacting with the negatively $SQ^-$ along its unbinding pathway.

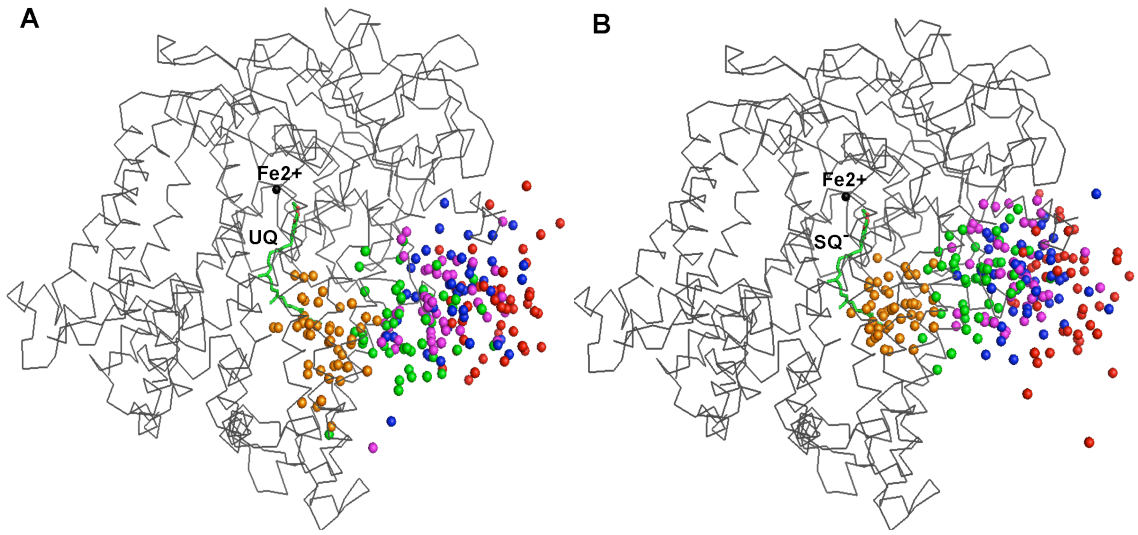


Figure S4: Position of the C29 quinone tail atom during unbinding for neutral UQ (A) and anionic $SQ^-$ (B) at five selected time points in the 45 SMD simulations. The positions are depicted by colored balls where each color represents a specific time point: orange (2000 ps), green (4800 ps), magenta (5800ps), blue (6400 ps) and red (8000 ps). The Fe2+ co-factor is shown as a black sphere and initial quinone position in green sticks.

Full list of authors for GAUSSIAN-98 software reference

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