Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Figure S1: Comparison of the electrostatic potential energy (V) and Fe-Fe separation (d_{FeFe}) for the hits from the Brownian Dynamics simulations for docking cyt b_5 with Mb(wt) and Mb(3M). Colored circles identify the starting geometries. Border plots show the total number of hits in a slices with V = 0.1 kcal/mol and d_{FeFe} = 0.1 Å.

Figure S2: A semi-log plot of average electronic coupling constants as a function of d_{FeFe}, colored according to whether or not a solvent molecule is found in the pathway (red) or not (blue). For reference, the fit line for the couplings is given (from Figure 4) with $\beta = 1.3 Å^{-1}$ (black line), as well as the best fit obtained from the starting geometries of the MD, without water (gray line, $\beta_0 = 1.45 Å^{-1}$).

Table S1: Ranges in d_{FeFe} for Mb(wt) and Mb(3M) ensembles.

Table S2: d_{FeFe}, pathways calculated T_{DA}^2 average from 51 snapshots, the standard deviations from 51 snapshots, and pathways calculated from the production run initial structure (without water molecules).

Table S3: Analysis of water molecules that are within 3.5Å of the propionic acids' oxygen for the COM BD initial geometries. Shown is the average number of water molecules (for 50 snapshots), as well as their location.

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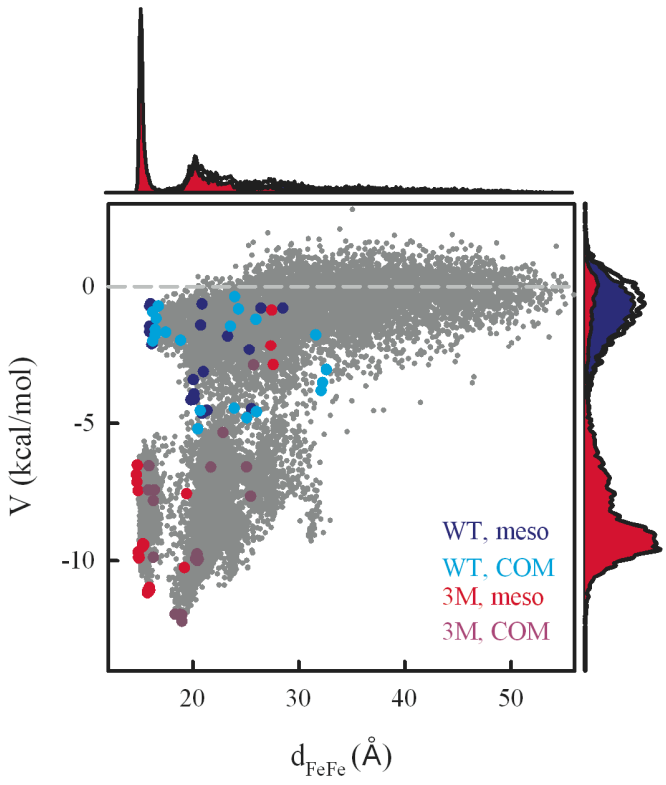

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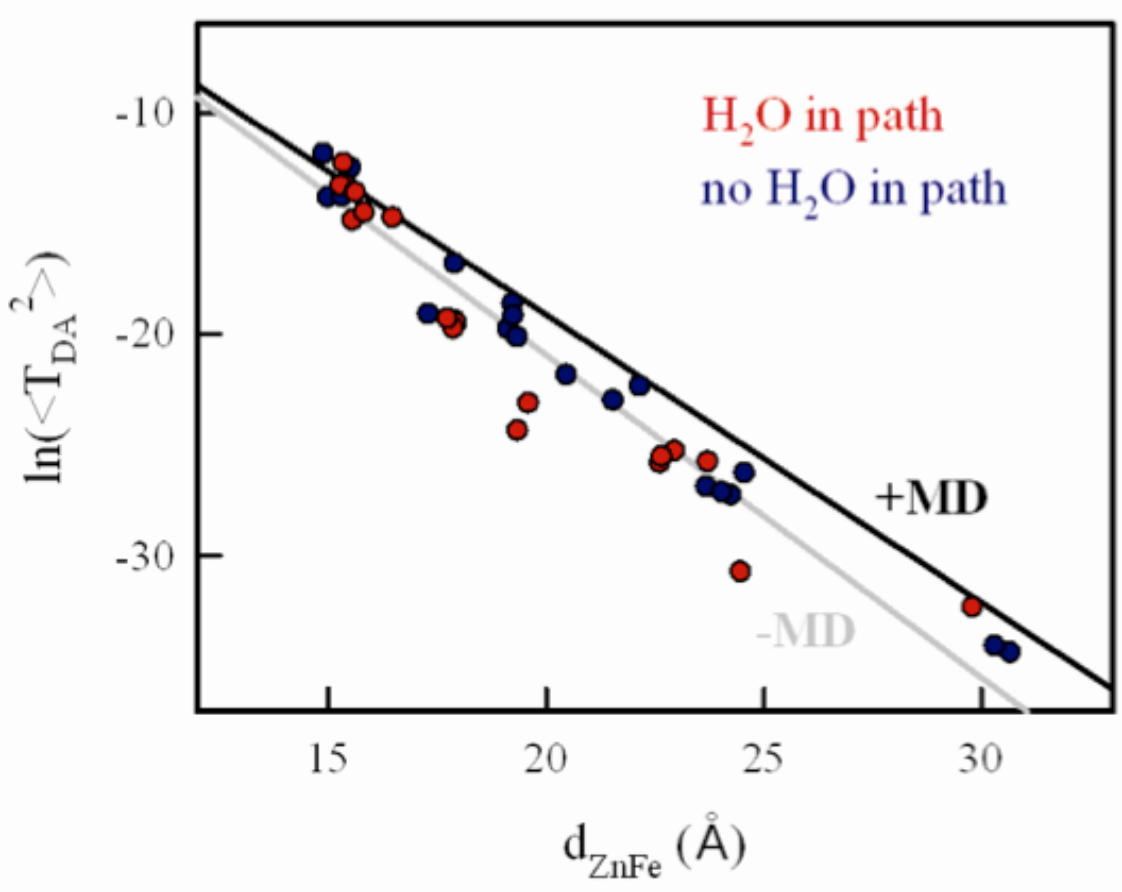

Table S1: Ranges in d_{FeFe} for Mb(wt) and Mb(3M) BD ensembles.

		d_{FeFe} (Å)	
		Minimum	Maximum
Mb(wt)	Meso-C	15.9	31.6
	COM	16.2	56.9
Mb(3M)	Meso-C	14.6	30.7
	COM	15.8	55.0

Table S2: d_{FeFe}, pathways calculated T_{DA}^2 average from 51 snapshots, the standard deviations from 51 snapshots, and pathways calculated from the production run initial structure (without water molecules).

	d_{FeFe} (Å)	$\langle T_{DA}^2 \rangle$ (eV^2)	std. dev. $\langle T_{DA}^2 \rangle$	${}^0T_{da}^2$
Mb(3M)	14.88	1.17×10^{-5}	1.27×10^{-6}	7.15×10^{-6}
	14.98	3.39×10^{-6}	4.80×10^{-7}	1.01×10^{-6}
	15.34	8.22×10^{-6}	1.04×10^{-6}	4.72×10^{-6}
	15.36	3.72×10^{-6}	4.46×10^{-7}	1.85×10^{-6}
	15.43	3.58×10^{-6}	4.77×10^{-7}	1.61×10^{-6}
	17.28	2.32×10^{-8}	3.47×10^{-9}	5.19×10^{-9}
	17.72	1.13×10^{-7}	3.89×10^{-8}	4.16×10^{-9}
	17.87	2.30×10^{-8}	4.65×10^{-9}	2.71×10^{-9}
	17.90	1.76×10^{-8}	4.22×10^{-9}	3.81×10^{-9}
	17.93	5.12×10^{-8}	1.76×10^{-8}	3.41×10^{-9}
	19.11	1.09×10^{-8}	3.30×10^{-9}	2.62×10^{-9}
	19.22	2.74×10^{-8}	9.71×10^{-9}	8.30×10^{-9}
	19.24	1.71×10^{-8}	2.83×10^{-9}	4.77×10^{-9}
	19.33	7.19×10^{-9}	2.10×10^{-9}	1.82×10^{-9}
	20.46	3.69×10^{-9}	4.44×10^{-10}	3.32×10^{-10}
	21.52	4.15×10^{-10}	7.99×10^{-11}	1.06×10^{-10}
	23.67	1.95×10^{-11}	4.22×10^{-12}	2.12×10^{-12}
	24.03	9.61×10^{-12}	4.07×10^{-12}	1.67×10^{-12}
	24.24	4.08×10^{-12}	7.86×10^{-13}	1.47×10^{-12}
Mb(wt)	15.28	4.65×10^{-6}	8.94×10^{-7}	1.72×10^{-6}
	15.29	1.98×10^{-6}	1.74×10^{-7}	1.05×10^{-6}
	15.51	6.45×10^{-6}	4.86×10^{-7}	3.79×10^{-6}
	15.55	9.12×10^{-7}	1.50×10^{-7}	3.60×10^{-7}
	15.60	2.27×10^{-6}	1.69×10^{-7}	1.26×10^{-6}
	15.62	2.49×10^{-6}	4.42×10^{-7}	1.25×10^{-6}
	15.81	1.33×10^{-6}	1.75×10^{-7}	5.10×10^{-7}
	16.47	1.29×10^{-6}	1.64×10^{-7}	4.05×10^{-7}
	17.89	2.53×10^{-7}	2.07×10^{-8}	5.10×10^{-8}
	19.34	1.09×10^{-9}	2.98×10^{-10}	2.71×10^{-11}
	19.58	4.54×10^{-9}	8.00×10^{-10}	9.31×10^{-11}
	22.13	1.32×10^{-9}	6.44×10^{-10}	2.00×10^{-10}
	22.60	5.83×10^{-11}	5.71×10^{-11}	6.31×10^{-12}
	22.63	4.98×10^{-11}	8.94×10^{-12}	8.32×10^{-12}
	22.94	6.67×10^{-11}	1.43×10^{-11}	1.08×10^{-11}
	23.70	3.34×10^{-11}	4.65×10^{-12}	6.64×10^{-12}
	24.45	4.79×10^{-12}	6.69×10^{-13}	4.63×10^{-14}
	24.55	2.97×10^{-11}	8.47×10^{-12}	3.93×10^{-12}
	29.78	2.18×10^{-13}	6.64×10^{-14}	9.41×10^{-15}

	30.30	9.94×10^{-15}	2.43×10^{-15}	1.65×10^{-15}
	30.56	2.06×10^{-15}	4.51×10^{-16}	4.28×10^{-17}
	30.66	4.74×10^{-15}	9.23×10^{-16}	1.22×10^{-15}
	30.65	5.18×10^{-14}	2.24×10^{-14}	5.07×10^{-17}

Table S3: Analysis of water molecules that are within 3.5Å of the propionic acids' oxygen for the COM BD initial geometries. Shown is the average number of water molecules (for 50 snapshots), as well as their location.

Protein	d_{FeFe} (Å)	Number of Water Molecules		
		Total	Mb side	Cyt b_5 side
Mb(3M)	14.9	24.0	18.0	12.0
	15.0	27.1	6.0	21.1
	15.3	41.1	20.1	27.6
	15.4	39.0	21.0	18.0
	15.4	39.0	21.0	18.0
	17.3	41.1	16.1	24.9
	17.7	46.5	18.0	28.5
	17.9	48.5	24.5	24.0
	17.9	45.1	21.1	24.1
	17.9	49.1	18.0	31.1
	19.1	47.4	14.6	32.8
	19.2	46.6	16.2	30.4
	19.2	47.3	22.4	24.9
	19.3	47.6	20.9	26.8
	20.5	57.9	21.8	36.1
	21.5	50.8	21.2	29.6
	23.7	31.7	3.2	28.5
	24.0	44.9	12.0	32.9
	24.2	36.9	9.2	27.7
Mb(wt)	15.3	34.9	16.9	21.0
	15.3	34.6	18.5	19.4
	15.5	39.0	15.0	24.0
	15.5	32.4	21.0	11.4
	15.6	35.8	17.6	27.2
	15.6	33.6	15.0	25.7
	15.8	44.1	23.1	27.0
	16.5	36.0	21.0	21.0
	17.9	41.9	18.0	26.9
	19.3	49.1	21.5	27.5
	19.6	54.8	24.5	30.4
	22.1	45.9	12.0	33.9
	22.6	47.4	17.6	29.7
	22.6	60.4	24.9	35.5
	22.9	53.1	21.0	32.1
	23.7	45.0	21.0	24.0
	24.5	54.0	23.9	30.1
	24.5	54.0	21.1	32.9
	29.8	54.4	23.4	31.0

	30.3	47.3	21.2	26.1
	30.6	51.6	23.1	28.6
	30.6	46.0	15.6	30.4
	30.7	49.5	18.1	31.4