Supporting Information

Perspectives on Electrostatics and Conformational Motions in Enzyme Catalysis

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M20C-CN and L28C-CN Probes

The main paper discusses two vibrational SCN probes (M20C-CN and L28C-CN) in Figure 4 of the main text that were not present in our previous publication on nitrile probes within the active site of DHFR (Ref. 10 of the main text). These data were obtained using analogous procedures and identical instrumentation to those of the original publication. The frequencies of maximum absorbance for all four probes in each of the five states along the DHFR catalytic cycle are provided in Table S1 below.

Table S1. Frequencies of maximum absorbance for SCN probes incorporated at four positions within the DHFR active site for five states along the catalytic cycle.

Ligands	Frequency of Maximum Absorbance (ν_{max}, cm^{-1})			
	M20C-CN	L28C-CN	T46C-CN	L54C-CN
E:$NADP^+$:FOL	2164.7	2160.4	2164.0	2162.1
E:$NADP^+$:THF	2156.3	2160.6	2159.9	2161.1
E:THF	2158.7	2159.9	2161.1	2160.9
E:NADPH:THF	2156.3	2160.9	2162.6	2160.6
E:NADPH	2161.3	2163.3	2168.1	2159.7