Supporting Information:
Eliminating imaginary vibrational frequencies in quantum-chemical cluster models of enzymatic active sites

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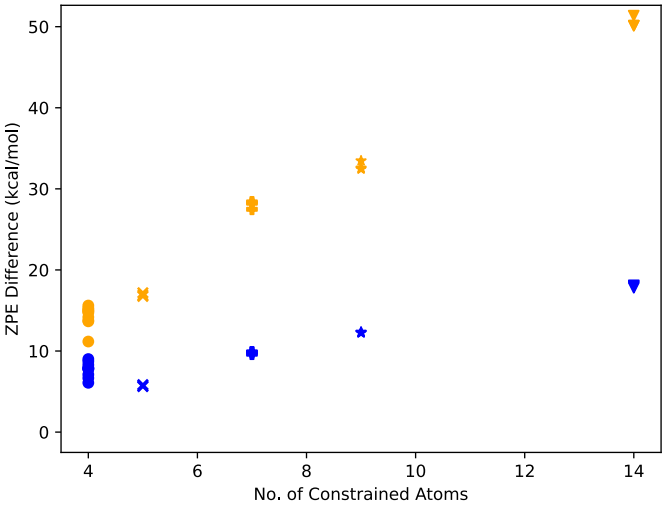

Figure S1: Difference in ZPE, relative to the unmodified Hessian with fixed-atom constraints, for a fixed-atom calculation with a zeroed-out Hessian (symbols in blue) and for models with harmonic confining potentials (symbols in orange), as a function of the number of anchor atoms. Circles on the far left correspond to the dipeptides in Table 1 whereas other symbols represent AspDC models I–IV.

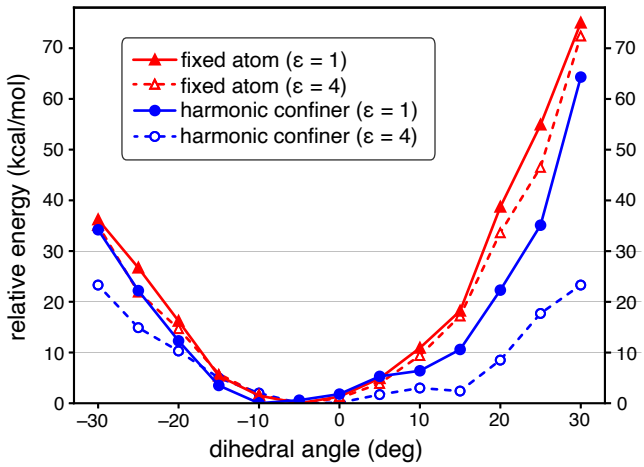

Figure S2: Relaxed torsional scans of ThrRS around the biphenyl dihedral angle that is depicted in Fig. 2, computed at the B3LYP+D3/6-31G(d,p) level using either vacuum boundary conditions ($\varepsilon = 1$) or else C-PCM boundary conditions with $\varepsilon = 4$. This is an overlay of the two panels that appear in Fig. 3.

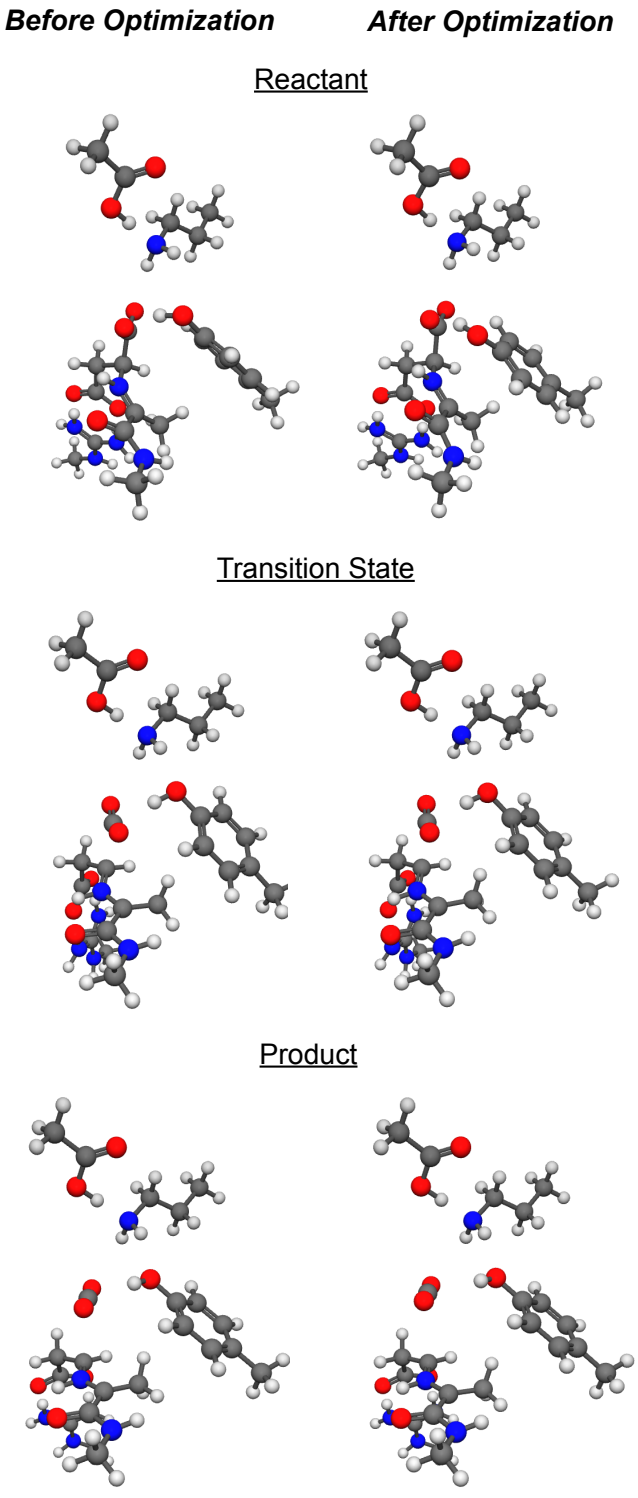

Figure S3: AspDC model I structures before and after optimization using the harmonic confining potentials. The "before" structures are taken from Ref. 1 and were optimized at the B3LYP/6-31G(d,p) level, whereas the "after" structures were optimized here at the B3LYP+D3/6-31G(d,p) level with harmonic confining potentials for the anchor atoms.

References

[1] Liao, R. Z.; Yu, J. G.; Himo, F. Quantum chemical modeling of enzymatic reactions: The case of decarboxylation. *J. Chem. Theory Comput.* **2011,** *7*, 1494–1501.